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**Ecotoxicological models for Dutch environmental policy**  
Models to be addressed in the Stimulation Program  
Systems-Oriented Ecotoxicological Research (NWO/SSEO)

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Directoraat-Generaal Rijkswaterstaat



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# Abstract

## Ecotoxicological models for Dutch environmental policy

Ecotoxicological models are one of the methods for judging the seriousness of environmental risks of contaminants in ecosystems. Such models range from very simple to complex. A simple model is the derivation of a generic quality criterion for a compound based on data collected in a laboratory toxicity test, using the lowest toxicity value and a safety factor. More complex models address variability between organisms, they concern laboratory-to-field extrapolations and/or they pertain to the biological features of the exposed organisms or systems. The Dutch national Stimulation Program Systems-Oriented Ecotoxicological Research (SSEO) aims to investigate the ecological implications of the ‘grey veil’ of contamination present in Dutch soils, sediments and surface waters. Within this program, this report concerns the first phase of the so-called Toolbox project. It provides an inventory of some models currently used for prospective and retrospective risk assessments. In phase two of this project, these models will be scrutinized as to their ability to accurately predict adverse effects in ecosystems. Validated models will be part of a “Toolbox” that will serve further policy formulation and risk management.

**Keywords:** eco(toxico)logical models, inventory, environmental policy, contamination, risk assessment.

# Rapport in het kort

## Ecotoxicologische modellen ten behoeve van het Nederlandse milieubeleid

Elk ministerie heeft zijn eigen modellen voor inschatting van risico's van stoffen. Dit rapport bevat een selectie van modellen die gebruikt worden om risico's voor planten en dieren te schatten.

De resultaten van veldmetingen worden vergeleken met normen. De laatste tijd is het aantal gevallen waarin milieunormen worden overschreden gegroeid. De volgende vragen moeten worden beantwoord:

Hoe erg is normoverschrijding? Zijn de normen streng genoeg, om effecten van mengsels van stoffen te voorkomen?

Het aantonen van effecten veroorzaakt door mengsels van verontreinigingen is moeilijk. Daarom is een onderzoeksprogramma opgezet: "Stimulerings-programma Systeemgericht Ecotoxicologisch Onderzoek" (SSEO).

In het SSEO programma zijn metingen verzameld op plaatsen met langdurige verontreinigingen met mengsels van stoffen in lage concentraties. De gemeten concentraties zullen in de volgende onderzoeksfase worden gebruikt om de toepasbaarheid van de modellen te onderzoeken. Er wordt nagegaan, of het beleid gelijk kan blijven of veranderd moet worden om de gestelde beleidsdoelstellingen kunnen halen.

**Trefwoorden:** eco(toxico)logische modellen, inventarisatie, milieubeleid, vervuiling, risicobeoordeling.

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## Samenvatting

In Nederland (en in de rest van de wereld) staat de biodiversiteit onder druk. Verontreinigingen vormen slechts één van de stressfactoren die de biodiversiteit kunnen aantasten. In welke mate dit gebeurt is niet duidelijk. Andere bronnen van stress zoals overstroming, verzuring, intensivering van landgebruik en habitat-fragmentatie kunnen de identificatie van de effecten van verontreinigingen voor de waarnemer bemoeilijken. Toch zijn er in Nederland grote aantallen locaties bekend waar verontreinigingen de lokale ecosystemen zouden kunnen bedreigen. Dit wordt verondersteld, doordat er op die locaties sprake is van concentratieniveaus van de verontreinigende stoffen boven de zogenaamde Interventiewaarde. Afgemeten aan overschrijding van de streefwaardes van diverse stoffen wordt ons land daarnaast gekenmerkt door de aanwezigheid van een “chemische deken” van diffuse verontreinigingen. Deze verontreinigingen kunnen deels van natuurlijke oorsprong zijn, zoals bij nutriënten en zware metalen, maar zijn grotendeels van niet-natuurlijke oorsprong zijn (xenobioten).

Het ecologische risico van de diffuse chronische stress van mengsels van diffuse verontreinigingen is niet bekend, maar kan wel beleidsmatig van belang zijn: het is namelijk niet eenvoudig om aan te tonen of- en in welke mate de “grijze deken” effecten veroorzaakt worden in ecosystemen, en of het beleid gelijk kan blijven, dan wel (deels) afgezwakt of geïntensiveerd zou moeten worden om de oorspronkelijk gestelde beleidsdoelstellingen te halen.

Vormen deze mengsels van verontreinigingen inderdaad een bedreiging voor de biodiversiteit? In hoeverre vermindert de verontreinigingsgraad het realiseren van algemene milieukwaliteitsdoelen, het bereiken van een ecologische hoofdstructuur van goede kwaliteit, of het behalen van de doelen van het waterbeleid?

Om de risico's van enkelvoudige verontreinigingen voor generieke soortenverzamelingen te bepalen zijn ecotoxicologische modellen ontwikkeld waarmee de onder laboratorium condities getoetste effecten van contaminanten geëxtrapoleerd worden naar waarschijnlijke risico's in het veld. De hierbij afgeleide wetenschappelijke risicogrenzen worden in de vorm van generieke normen toegepast in wet en regelgeving.

Doordat het aantal gevallen waarin de normen worden overschreden in de loop der tijd steeds verder gegroeid is, is de vraag dringend geworden hoe realistisch een via normoverschrijding vastgestelde schatting van de risico's voor ecosystemen is. Deze urgente en breed levende vraag, en de technische problemen rond het aantonen van diffuse chronische veldeffecten veroorzaakt door een mengsel aan verontreinigingen, heeft er toe geleid dat het “Stimuleringsprogramma Systeemgericht Ecotoxicologisch Onderzoek” (SSEO) is opgezet. Dit programma opereert onder auspiciën van de Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO). Het SSEO-programma heeft de volgende doelstellingen:

- Het verzamelen van wetenschappelijke data rond de responsies van ecosystemen op chronische en diffuse chemische stressoren. Dit vraagt om causaal-analytisch onderzoek naar de relatie tussen stressoren (waaronder mengsels van stoffen) en populatie en systeemeffecten in het veld.
- Het gebruik van de verzamelde wetenschappelijke inzichten ten behoeve van de beantwoording van de vraag hoe om te gaan met chronische en diffuse stressoren,

ofwel voor het formuleren van veld-relevante ecologische risicobeoordelingsmethoden voor praktisch gebruik. Na een grondige beleidsevaluatie kunnen de resultaten van het programma leiden tot bijstelling van het risicobeleid.

Het SSEO programma (2000 - 2006) heeft dus als primaire doelstelling om de implicaties van blootstellingsscenario's te bestuderen in biotische leefgemeenschappen onder veldcondities. In het programma wordt de nadruk gelegd op de "grijze deken" veroorzaakt door mengsels van verontreinigingen met relatief lage concentraties. Dit wil zeggen, concentratieniveaus die de kwaliteitsnormen (Streefwaarde) overschrijden, maar waarvoor geen duidelijk aanwijsbare effecten op de biotische leefgemeenschap waarneembaar zijn. Wanneer de implicaties van de "grijze deken" beter bekend worden, kunnen de tot heden gebruikte ecotoxicologische risicomodellen op dergelijke gegevens (verder) gekalibreerd worden. Eveneens kan de ontwikkeling van methodieken voor locatiespecifieke risicobeoordeling hiervan profiteren. Dit zal leiden tot meer accurate risico-inschattingen van effecten in het veld: zullen er op een verontreinigde locatie effecten optreden, en zo ja, in welke mate? Validatie van de tot heden toegepaste eco(toxico)logische risicomodellen is van groot belang, gezien het feit dat onderschatting van effectnormstelling een ongewilde milieuimpact teweegbrengen, terwijl overschatting van effectnormstelling veel geld kost waarbij het milieu niet optimaal baat heeft.

Elk ministerie heeft voor het beheersen van de risico's van stoffen een eigen aanpak, die ontwikkeld is in het licht van hun eigen verantwoordelijkheden, respectievelijk voor algemene milieukwaliteit, voor soorten uit het natuurbeleid, of voor waterkwaliteit. Risicobeheersing kan gebaseerd zijn op een generieke aanpak of op een locatie-specifieke aanpak, en kan variëren van preventief tot curatief. Het afleiden van een generieke kwaliteitsnormen voor algemene milieubescherming is een voorbeeld van een preventieve, stofgerichte aanpak. Onderzoek naar de populatiebiologie van bedreigde soorten die onder toxische stress staan is een voorbeeld van specifiek georiënteerde aanpak. Gebaseerd op de specifieke beleidsproblemen wordt in dit rapport een selectie aan onderliggende risicobeoordelingsmodellen beschreven.

Dit rapport is gemaakt in het kader van het laatste project van het SSEO-programma. Dit project richt zich op modellen, hun relaties met de beleidsvragen en hun relaties met de via het SSEO-programma verzamelde gegevens over effecten in het veld. In dit project werken de instituten Alterra, Radboud Universiteit Nijmegen, RIZA en RIVM samen om:

- In fase 1: een lijst op te stellen van modellen die het Nederlandse milieubeleid ondersteunen

- In fase 2: te onderzoeken in hoeverre deze modellen gevalideerd kunnen worden aan de hand van data gegenereerd/verzameld door de andere partijen in het SSEO programma.

Het huidige rapport bevat de (beperkte) lijst van geselecteerde modellen, zoals genoemd voor fase 1. De werkzaamheden voor fase 2 worden ten tijde van het vaststellen van dit rapport uitgevoerd.



## Summary

In the Netherlands (and elsewhere) biodiversity appears to decrease at many sites and in many ecosystems. Pollution is just one of the stress factors that may threaten biodiversity. It is unclear to what extent pollutants are indeed a threat to biodiversity. Other sources of environmental stress such as inundation, acidification, intensive land-use and habitat fragmentation make the effects of pollutants difficult to proof. Nonetheless, Dutch ecosystems at a large number of sites may suffer from pollution. This is an expectation that is based on the observation that at those sites the Intervention Value is exceeded. The country is, as judged from exceedances of the Target Values, also covered by an apparent (so-called) “chemical blanket”; a diffuse chemical load consisting of a range of different contaminants. These contaminants can vary from ones with a natural origin, e.g. nutrients and heavy metals, to ones that are xenobiotic.

Due to the large numbers of exceedances of lower or higher risk limits, it has become crucial for risk management and environmental policy to determine the real ecological risks of especially this diffuse, chronic stress caused by mixtures of contaminants, especially when considered in combination with other environmental stress factors. Is there evidence to conclude that the policies can remain similar, or are there reasons to intensify or reduce the risk management efforts after considering true toxicant effects in the field? Is this mixture of contaminants indeed a threat for biodiversity? To what extent does an environmental mixture of contaminants reduce the realization of a good environmental quality in general? To what extent can realization of the Ecological Main structure be expected? And to what extent can a good ecological quality of the Dutch surface waters be expected?

For single substances, ecotoxicological models are in use to extrapolate single species laboratory toxicity data on pollutant effects to higher levels of biological integration. Model results addressing such effects are used to derive compound-specific risk limits and these are translated to generically applicable environmental quality criteria. Results of other models are used to assess location-specific risks on target populations of red list species.

Since it became more and more obvious from various inventories that the quality criteria are frequently exceeded, it became more and more an intriguing problem to ascertain that diffuse, chronic stresses caused by combinations of contaminants indeed trigger adverse, undesired ecological effects. In turn, this question triggered the development of the Stimulation Program Systems-Oriented Ecotoxicological Research (in Dutch “Stimuleringsprogramma Systeemgericht Ecotoxicologisch Onderzoek – SSEO). This program operates under the auspices of the Dutch Organization for Scientific Research (NWO). This program has the following objectives:

- To gather scientific data on ecosystems' responses to chemical stresses of a chronic and diffuse nature and to analyse the causal relationship between low-level chronic mixture exposure and effects on populations and ecosystems in field conditions;
- To use the collected knowledge for formulating and implementing risk management policies for handling chronic and diffuse exposure of the environment to mixtures of contaminants.

The SSEO program (2000 - 2006) aims to study the implications of the exposure of biotic communities in field conditions. Emphasis in the program is on the hypothesized “chemical blanket” that consists of mixtures of contaminants at relatively low concentration levels. That

is, levels that do exceed the generic quality criteria, but (at first sight) do not apparently induce obvious adverse effects to biotic communities. When true effects of “chemical blanket” exposure would become more clear over time, the ecotoxicological models used in the derivation of the criteria can be calibrated or validated by using those data. In addition, the development of site-specific risk assessment methods may profit. Both will eventually lead to risk management decisions that are improved by knowledge of the probability that field effects are likely to occur and of the magnitude of effects that is likely. Calibration and validation of commonly used models are of major importance, since under-protective criteria imply undesired environmental impacts, while over-protective criteria imply that money is spent without environmental benefit.

In view of their responsibilities for their own policy fields, ministries have developed approaches that are tailored to the specific problems they have to handle. Environmental policies are based on generic approaches or on location-specific approaches and range from preventive to curative. The derivation of generic quality criteria for general environmental protection is an example of a generic, preventive, compound-oriented policy. Investigations into the population development of endangered species under toxic stress are an example of a species-oriented approach. Based on the specific set of policy problems, this report describes a selection of the underlying set of models and how these models link to the policy problems.

This report has been prepared as last project of the stimulation program, SSEO. The project focuses on models, their relationships with policy problems and their relationships with true effects as compiled in the other SSEO-funded research projects. In this project, the institutes Alterra, Radboud University Nijmegen, RIZA and RIVM work together to (subsequently):

- In phase 1: list a set of models supporting environmental policies in the Netherlands and
- In phase 2: investigate the degree of validation of those models with the data collected by other parties in the SSEO program.

This report concerns the (limited) listing of the selected model, as mentioned for phase 1. Phase-2 research has started.

# 1. General introduction

## 1.1 Risks and environmental policies

Chemical compounds are emitted into the environment, due to human activities. These compounds may cause adverse effects on man and ecosystems. This fact has triggered national governments to develop risk management policies. This concerns both general environmental policies (general protection) as well as targeted policies (specific protection), e.g. for compartments (water, soil) or for specific endpoints, like nature policies. The target of those policies is to avoid reductions of environmental quality and to limit and reduce risks of toxic compounds.

In the Netherlands, Europe and elsewhere, these policies were initially founded upon a fundamental choice. Namely, to choose for a risks-based approach, see e.g. VROM (1988) and Van de Meent et al. (1990). This was done to create methods for risks and effects reduction by either preventive or curative risk management activities. The use of a risk-based approach in environmental policies has been advocated by the following motives, from Suter (1993):

1. (formal) risk assessments require an explicit identification of policy protection or remediation targets; these are the starting point for any risk assessment
2. they require clear definition of approaches and assumptions of the risk assessment process, to yield a clear background for discussions in the management of (different) risks
3. they require a clear distinction of roles between the (scientific) process of risk assessment and the (policy) evaluation of risk management
4. they are a systematic basis for better recognition and understanding of the occurrence of risks and effects
5. they allow for the comparison of risks induced by different stressors and for priority setting in risk management
6. they show the explicit uncertainties that are embedded in the forecasting of events

Environmental risk assessment by modelling is an important basis for the regulation of toxic compounds. Modelling can, however, yield good or bad results. When there are large implications at stake, such as large investments that are made for risk management, it is relevant that those model results accurately predict true effects. Calibration of model results to effect data and/or validation of the models are of societal importance, since e.g. costs of sanitation measures are large.

## 1.2 Definition of risk and risk modelling

Risk analysis is central to chemical regulation policies, but what is a risk exactly? Risks are generally defined on the basis of both the probability of exposure of so-called receptors (exposed organisms) and the sensitivity of those organisms to exposure. Together, the ratio of exposure over sensitivity determines the likeliness and magnitude of effects. The quantification of risks is thus by definition a process that involves *modelling*. Risk is a concept most often concerned with future events (*prospective risk assessment*) and is not a directly observable phenomenon – effects are observable, risks not. In so-called *retrospective*

*risk* assessment, one considers e.g. a contaminated ecosystem and tries to quantify local risk, so as to support decision making. Thus, risk assessment involves at least one modelling step, determining by simple or complex calculations the ratio of the exposure probability over the magnitude of effects.

A simple “model”, used to derive generic environmental quality criteria (EQC) for compounds for which data are scarce, is the use of laboratory toxicity data for the most sensitive species and divide the resulting value by an uncertainty factor. More complex models address variability amongst organisms and in exposure conditions and may make use of specific ecological features of organisms. An example of the latter is the quantification of likely effects of toxicant exposure using population models that are based on age-dependent birth- and death-rates and thus on the biology of species.

In general, exposure and effects can be modelled or measured. Exposure levels, for example, are dependent on the distribution of compounds in the environment (resulting from emission patterns and the physico-chemical properties of the compound). The underlying processes can be captured in fate models. Effects are usually difficult to determine in the field and are modelled by assessing a sensitivity pattern for the exposed organisms or organism groups from laboratory data. Extrapolations are often needed to translate the observations collected in laboratory studies to field situations. As a net result of all efforts made so far, formal risk assessment procedures have been developed and adopted to assess the possible risks linked with the emission of toxic compounds. Ecotoxicological modelling has thus been applied for many years. An array of models is available to address different types of risk management questions. Note that two output types are common, namely (1) quality criteria (fixed numbers, mainly used in a preventive context) and quantitative risk values for contaminated sites (a curative context).

### **1.3 Current challenges of risk-based decision making**

Despite the general use of models to support environmental policies, the model outcomes are currently strongly challenged in view of the current state of the environment. In the Netherlands, for example, the current status of the environment is generally considered to be deteriorated for large areas, with huge numbers of ‘hot spots’. For sediments, inventories on the sediment quality in Dutch surface waters have shown a large workload of contaminated sediment to be handled (AKWA, 2001). Clean-up would imply huge financial investments and many stakeholders would be involved. A major policy question is how to balance between safe water management and safe sediment removal and deposition elsewhere.

For terrestrial soil, inventories in the framework of the action “Landsdekkend Beeld, Spoor 1”, see e.g. (Kernteam Landsdekkend Beeld 2004) have shown that (status March 2005) a few hundreds of thousands of sites may be contaminated above the concentration level of the Intervention Value. This view was constructed from on inventories of past activities, extended with expert knowledge of the contamination levels to be expected. According to the current views, it is estimated that approximately 350.000 – 400.000 sites might require further local research and that eventually, say, 60.000 sites might be listed for obligatory sanitation.

Next to these two sets of workloads, there is of course also the exceedance of the lower quality criteria, the Maximum Tolerable Risk (MTR) and Target Value (TV) levels, to be addressed in the near future in a further inventory, the action “Landsdekkend Beeld,

Spoor 2". For these lower-level criterion exceedances, the ecological impacts on soil, sediment and aquatic ecosystems are largely unknown. They are not known from inventories on field effects and they have not systematically been predicted by risk modelling.

All abovementioned workloads are examples of the magnitude of the environmental contamination situation in the Netherlands and pertain to general environmental quality (special responsibility: VROM), water quality (special responsibility: V&W) and nature policies (special responsibility: LNV).

As a consequence of the inventories compiled above, both the government itself and the stakeholders are questioning whether exceedances of the generic quality criteria imply the presence of effects on ecosystems in the field. Because the inventories make use of generic quality criteria to identify cases as part of the workload for sediment management or soil sanitation and since these are in turn based on risk modelling results, a major question has thus emerged:

***What does exceedance of quality criteria mean in terms of effects on biota in the field?***

This question is posed more frequently today than in the recent past.

Posing the question implies that there are two distinctive ways to look at the environmental problems on the basis of risks and risk modelling, as shown in Figure 1. For the derivation of generic quality criteria, there is the potential hazard posed by the intrinsic characteristics of the compounds that might be emitted into the environment. For those compounds, one collects dose-response data and (by extrapolation) one can characterize risk profiles. When limits are set (by policy choice) on the tolerable level of risk, the risk profile curve can be used to set ambient exposure concentrations that are considered safe, or that trigger remedial action. These values are known as the abovementioned environmental quality criteria. For retrospective risk assessments (of contaminated sites), the same model concepts hold, but in a different order and without the idea of a pre-set cut-off criterion. The result of a retrospective assessment is a quantification of a local level of risk or impact (risk characterization), which is the basis for a site-oriented risk management decision (such as clean-up, site management activities, or no action). It is expected that the second type of risk assessment becomes more prominent over time, both in The Netherlands (e.g., VROM (2003), partly due to investigations on pollution hot spots (Kernteam Landsdekkend Beeld 2004)) as well as in Europe (e.g., Risk-Based Land Management).

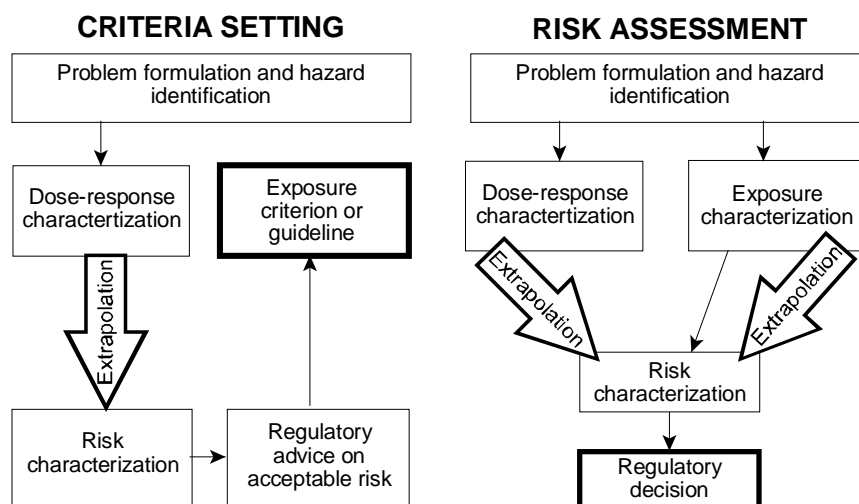


Figure 1. The two perspectives on the use of risk modeling in environmental management of toxic compounds

## 1.4 Addressing risks from various perspectives

Answering the key question posed above is not easy. Although it is often obvious that a calculated risk level is substantiated by (easily) discernable effects on exposed biota at *high* contamination levels, the question is more difficult to answer whether calculated risk levels predict true effects in the field at *low* exposure levels.

From a generic perspective, e.g. seen from the general environmental protection responsibilities of VROM, is there a clear association between exposure and effects in the field? How are risks “substantiated” in the format of ecological responses? An array of sub-questions can be posed, such as:

- What does a relatively small exceedance of risk limits imply for the exposed biota?
- How does a combination of single compounds of which some exceed and some are below risk limits affect biota in the field?
- What is the influence of other environmental stress factors on the sensitivity of biota for pollutants?

When looking at more specific policies, questions are emerging also in e.g. compartment-oriented or nature-oriented policies. For example, nature policies are directed at the protection of biodiversity in specific areas (e.g. Natura 2000 sites related to the Ecological Main Structure, Ecologische Hoofd Structuur) and at protection of threatened species (see, e.g., the Habitat and Bird Directives and species protection plans). These policies aim at maintaining species or habitats and biodiversity in general in a good conservation status. Within the latter policies, toxicants are only one of a range of stress factors that may have a negative impact on the conservation status. Nature policies do not include specific guidelines for stress factors such as toxicants but take these into account when evaluating the conservation status of its objectives. The assessment of impact is usually more evaluation-based than risk-based *per se*. As in the more general environmental policies, models play a mayor role in the area and species assessments. Evaluations on how chemical compounds can decrease the viability of species and the integrity of habitats and biodiversity can in this case only be achieved by using (complex) models to interpret measurement made on exposed

populations. In the Netherlands the role of toxicants on biodiversity is often considered minor compared to other stress factors such as habitat loss, eutrophication and acidification. In the European context, toxicants are, however, specifically mentioned as an important factor (see e.g. the Habitat Directive). Given the large amount of sites in the Netherlands with relatively low levels of toxicants (to be quantified and qualified by “Landsdekkend Beeld Spoor 2”) the question is to what extent these substances threaten biodiversity in general and objectives of nature policies specifically.

## 1.5 Systems-Oriented Ecotoxicological Research

The *Stimulation Program on Systems-Oriented Ecotoxicological Research* (in Dutch: SSEO) was established to address the above types of problems. The program aims:

- to collect scientific insights in the field effects of contaminant mixtures at low to moderate exposure levels on local biota and
- to interpret these insights as to furthering the understanding of the meaning of the ‘grey veil’ of contaminants that is apparently present in the Netherlands, so as to (eventually) derive implications for risk management policies.

The SSEO-program is funded by various ministries and NWO<sup>1</sup> and is currently being executed by an array of research groups. Each of these groups works on one of three selected field sites, on the fate of contaminants at those sites and on the quantification of effects in various organism groups. In the program, the focus was placed on system-level ecological effects, to be determined whenever possible under field conditions.

The central aim of the program is:

***To gain scientific insight in the risk of chronic exposure of ecosystems to a combination of pollutants, in order to (eventually) improve environmental management of toxicants***

To improve on the insight on the problem, three suitable research locations were selected by specialists, which offered a set of research parameters that would be needed for applying existing ecosystem models. The locations were evaluated on the basis of criteria such as existing information on ecology, chemistry and toxicology, possibilities to study a gradient in pollution and relevance to risk management policies. The list of preferred ecological parameters ranged from single species population parameters to more complex ecosystem function parameters.

To further the improvement of environmental management, the program asked for attention for the set of models that is used and applicable in the environmental policies. Specifically, the SSEO-integration project was started to collect, describe, validate and evaluate the current use and possible future use of those models.

Regarding the SSEO-integration project, two phases can be distinguished:

1. The inventory phase, in which modelling experts compile a set of models while the other SSEO-researchers compile their field data;
2. The validation phase, in which the modelling experts and the other researcher collaborate in added data analyses, i.e., to investigate the validity of the different models when confronted with real field data.

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<sup>1</sup> NWO=Dutch Organization for Scientific Research

Within the first phase also incidental advices of modellers to site researchers is given, in order to improve the fit between measured parameters and required model parameters. The second phase also consists of integrative activities, whereby separate data sets of different researchers are compiled, making calculations possible which could not be performed with the separate data sets.

## 1.6 Aims of this report

The objectives of the research for this report (first phase) are:

- To provide an overview of selected major environmental policy problems associated to the distribution of toxic compounds in the environment;
- To list and provide a current characterization of the ecotoxicological models associated to those problems

This research will be extended within a year in a second report (second phase) within the SSEO-program context (the validation of the models with field data). In that phase, the following objective is added:

- To provide the basis for a decision-support toolbox for environmental management purposes assembled from existing ecotoxicological effect models, including a set of guidelines that instruct users when and how to use certain tools and how to interpret their output, including explicit use limitations.

Note: this report addresses only the first phase and thus provides an overview of the policy problems for which models have been used and are used and the pertinent set of models. The validation question is only addressed on the basis of some existing examples, but this question will mainly be addressed the second phase.



## 2. Current approaches in risk management of toxicants

### 2.1 Overview

The Ministries involved in policy formulation for toxic compounds are the Ministry of Housing, Spatial Planning and the Environment (in Dutch: VROM), the Ministry of Agriculture, Nature Management and Food Safety (in Dutch: LNV) and the Ministry of Transport, Public Works and Water Management (in Dutch: V&W). In this chapter some illustrations of the risk management problems of these ministries are given. It is shown how the policy problems link to the issue of modelling and via modelling and model validation by field data, to decision making. Moreover, we show that models are used in the pertinent policies and that these models are linked by underlying modelling principles and protection targets. This chapter is aimed to be illustrative and challenging for those active in risk management and policy making and not to contain a complete overview of all risk management problems.

### 2.2 Linking protection endpoints, models and field effects

#### 2.2.1 General

Although it would seem obvious, policy problems can usually not be directly translated to effects in the field (see Figure 2). Policy problems like the contaminant risk problem usually provides a general notion of protection or clean-up targets, this notion not necessarily being clearly defined and operational for testing. The latter is needed, since one cannot otherwise derive management rules to be applied in practice, nor can one see whether the policy targets are reached (e.g., “distance to target” methods and the principle of *From Policy Planning to Policy Account*).

Scientific analysis of the policy target is commonly needed to propose an operational measure to enable quantification of the target in measurable units (compare: a ‘ruler’). On this ruler, (risk) limit values are assigned to discriminate between policy-unacceptable and policy-acceptable risks. This discrimination should be informed by knowledge of affected systems, so that in the ideal case the discrimination between unacceptable and acceptable effects is exactly linked to the policy target, via the risk ruler.

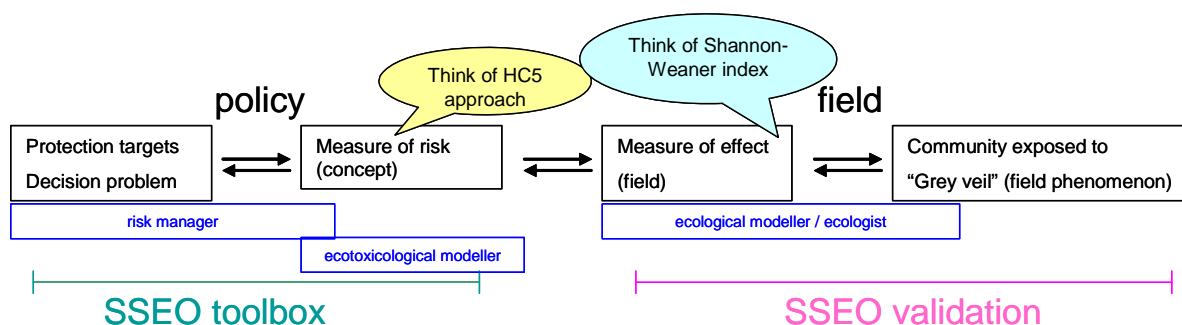


Figure 2: Stepwise linkage between policy problem, models and field effects

In the first block, a decision problem is encountered by the policy makers. As an example, for the case of contaminant risks, generic protection targets have been formulated, with the specific notion of ecosystem protection being integrity of structural and functional characteristics. In this case, one of the pertinent rulers (e.g., that for structural integrity) has been developed in the basis of the Species Sensitivity Distribution (SSD) model, yielding the generic risk limits on the ruler that are known as HC5<sup>2</sup> and HC50, which are the ecotoxicological foundations for the Target (HC5/100) and Intervention Value (=HC50) in policy, respectively, see e.g. (Sijm et al., 2002). These modelled risk limits were introduced in the late 1980s (Van Straalen and Denneman, 1989) and in the 1990s (Swartjes, 1999), for the lower and the higher limit values, respectively, under the assumption that the HC5 and the HC50 are linked to real field effects: no unacceptable at the HC5 level and unacceptable exposure, triggering investigations into the need for remediation, at the HC50 level.

After the introduction of the idea and the application of the model in derivation of both criteria in practice, validation approaches were undertaken. Examples are provided by, e.g. Emans et al. (1992) and Okkerman et al. (1993) for the aquatic compartment and Posthuma et al. (1998), Posthuma and Smit (1999) and Posthuma et al. (2001) for the terrestrial compartment. All these studies suggested that the No Observed Effect Concentration of exposed communities (NOEC<sub>Ecosystem</sub>) was lower than the model-derived HC5. This supports the view that the HC5 and HC5/100 offer sufficient protection. Note that the NOEC<sub>Ecosystem</sub> itself is, again, a model result. It is derived by modelling from the set of raw field data. Various approaches can be chosen to translate those data into the measures of effects chosen in the validation studies, see e.g. Smit et al. (2002). The terrestrial studies, moreover, showed that the model-derived HC50 was associated with observable effects on biodiversity, or that it indicated a concentration where clear biodiversity effects were occurring at little extra exposure (Posthuma et al. 1998). These studies supported the view that the HC50 indeed indicated a level of serious concern, sufficient to consider remediation needs further. Note that the validation studies mentioned so far only touch upon *point estimates* on the risk ruler (HC5 and HC50), not on the whole SSD. The latter is the subject of current studies (see Appendix 1).

### 2.2.2 Using this approach in the second-phase of this project

Figure 2 can especially be used to illustrate the upcoming second phase approach of the SSEO-integration project. The SSEO-phase 1 research data pertain to the study and interpretation of field exposure and effect data into measures of field effects (fourth and third block) and is executed by many researchers. This interpretation asks for activities of ecologists and ecological modellers, the latter to translate the field effects in measures of effects (the “field-effect ruler”). The risk-modellers role was the design of a ruler for measuring risks. The final role is, evidently, to link the measures of risk to the measures of field effects. This is the abovementioned validation step.

When all this is done, the original risk management problem is linked to field effects on a local scale and the models and approaches used so far can be evaluated as to their efficiency in preventive and curative policies. The Figure and the example show that models are, in fact, often needed at two spots in the stepwise linkage between policy target and field effects. The first spot is the definition of a ruler associated to a policy end point, the second is the derivation of measures of effect from the field phenomenon.

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<sup>2</sup> HC=Hazardous Concentration, the number refers to the number of species likely affected

## 2.3 The functions of models – and alternative approaches

Models can be of help for the following issues and these functions are explicitly related:

- making a potential environmental problem *visible*
- making the potential impacts *measurable*, at least in a relative sense that is sufficient to policy decisions and
- allowing for the *interpretation* of (relative) risks against the protection endpoints, as basis for policy formulation

An example of large-scale environmental monitoring is used to illustrate the function of models in the process. First, field inventories (nationwide monitoring) have shown that many sites and systems in the Netherlands are exposed at exposure levels that exceed the quality criteria (see section 1.3). Since the quality criteria are themselves, at least in part, model results (see Figure 2), it can easily be concluded that models play a key role in showing the presence of a problem. Monitoring of exceedance of the criteria has shown that policies might need to be refined, reduced or intensified. The problem has become *visible*.

Second, monitoring yields huge data sets that need to be interpreted. Thousands of sites, near a hundred thousand compounds and all different types of ecosystems complicate obtaining a comprehensive view. By applying the models again, usually better tailored to the problem, the monitoring data can be interpreted in terms of the number of times a quality criterion is exceeded for every separate compound. This is a simple form of post-monitoring modelling of large data sets, to facilitate interpretation. The statistical models used for the derivation of the quality criteria can, however, also be of help to summarize the set of data further, to a single value for toxic pressure for whole mixtures. An example of the re-shaping of a large monitoring data set, through modelling, in an easily interpretable format to support risk management decisions is provided in Appendix 1. In other words: the problem is *measurable* in terms of the model ruler and the protection target.

Third, by calculating integrative measures of toxic pressure by mixtures through modelling (e.g., the msPAF<sup>3</sup> of a mixture, see section 0), or the prediction of population viability under toxic stress (see section 4.3.3), one can analyze trends and impacts in the load of toxic compounds in the environment over time. Policy makers can find out whether there is a general response to their prevention policies, or how effective these policies are in reaching the target. Reaching the generic policy target of environmental “improvement” would show up as a downward trend in the integrated (modelled) integrated monitoring parameter over time. Reaching the target for species protection would show up as a reduced change of local population extinction for protected red list species. Hence, modelling can eventually help to translate a policy problem into endpoints that can be calculated from the monitoring data, which implies *interpretation*. With an appropriate interpretation, the outcomes can be used to intensify preventive policies, e.g. when an upward trend would show up from the monitoring data.

Note that the arguments provided here for the sake of modelling do *not* imply that modelling is the sole way to derive environmental management decisions. Targeted measurements, e.g., according to a weight-of-evidence approach, or sole bioassays or field observations, can be of equal help (see further section 5.1). The sole message given here is that, due to the complexity of the item and past decisions on using risk-based approaches for policy, models

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<sup>3</sup> msPAF=multi-substance Potentially Affected Fraction of species

are intricately coupled to the issue of toxicant-oriented policies (but not necessarily the sole solution).

## 2.4 Protection targets of generic environmental policies

As mentioned, there is a wide array of policies in which toxic compounds play a role, either as subject of the regulatory action itself, or as subordinate part of an integrated approach. This section describes a selection of current policy items for the different Ministries, thereby trying to describe protection (or remediation) targets in policy terms, the risk “rulers” that link to those targets and (when possible) some focus on the validation of the risk ruler to the field effects to be protected against.

### 2.4.1 Setting (Inter)national Environmental Quality Criteria (INS)

The VROM-Department for Toxic Compounds, Wastes and Radiation, VROM/DGM-SAS, is responsible for development and implementation of Environmental Quality Criteria (EQCs) for toxic compounds. An array of Dutch (government) research institutes and various stakeholders are involved in the derivation of EQCs (via the project INS, in Dutch: “Internationale Normstelling Stoffen”). The protection targets are broadly defined and concern a prevention against adverse effects of toxic compounds on humans and ecosystems.

There are various EQCs. The criterion known as the Maximum Tolerable Risk (MTR) and the Target Value (TV) are used to assess the general environmental quality. MTR indicates the quality level that should soon be reached. When reached, the TV becomes the endpoint of the policy. The TV identifies the quality level that should be reached on the long term. In the National Environmental Policy Plan, the target dates are 2000 and 2010 for reaching MTR and VR, respectively.

EQCs are used for various purposes:

- Firstly, emission-oriented policies are formulated based on MTRs and TVs and priorities are set within these emission-oriented tracks. Exceedance of MTRs is an important indicator for source-oriented risk management action. MTRs for sediments are used to derive source-oriented measures, especially for those compounds that strongly sorb to sediment. For dry soils, the MTR-criterion has not been adopted for source-oriented policies, since the improvement of soil quality will not proceed as quickly in soil as in water.
- Secondly, until shortly, sanitation and remediation policies for soils and sediments aimed at clean-up till the TV was reached. When adopted, clean-up targets will in the near future likely be related to the local soil use (function-oriented sanitation, using Soil-Use dependent criteria, in Dutch: “Bodem Gebruiks Waarden”, BGWs)).
- Thirdly, emission permits are primarily released on the basis of EQCs. For the aquatic compartment, this process is extended by post-emission measurements on the occurrence of effects. If effects do occur despite the prediction that they are unexpected, further emission reduction is requested. Starting point in the evaluation of emission permits is that the emission may not significantly contribute to the exceedance of the quality criteria (MTR, or a specific, function-related value) for the water/sediment system (i.e., no acute effects in the mixing zone for neither water nor sediment inhabiting species). A special case exists for the admission of plant protection products on the market. For these compounds a specific tiered system is in use in both The Netherlands and the EU. In this tiered approach, absence of effects in

higher tier field studies results in registration of the compound, even when lower tier risk assessment would not exclude unacceptable effects.

In case formally adopted EQCs lack, the evaluation of the environmental quality as well as for the priority setting in managing emissions and sources and for the further demands that can be imposed in the case of specific point sources, the use of *ad hoc* MTRs is warranted. The models that are used in the INS-setting are compiled and explained in Traas (2001) and later protocols. Amongst others, the Species Sensitivity Distribution model is applied to derive the EQCs.

#### **2.4.2 Nature policies**

Nature policies can be divided in policies directed at protection of habitats and biodiversity in designated areas (Nature Conservancy Act, Ecological Main Structure, Birds- and Habitats Directive and its Natura 2000-sites) and policies directed at protection of species (Birds- and Habitats Directive, Flora and Fauna Act, Species Protection Plans, Red lists (national), Bird directive, Red lists (international)). See section 2.5.3 for a more in dept discussion on these policies. The policies can be further divided into national (Nature Conservancy Act, Ecological Main Structure, Flora and Fauna Act, Species Protection Plans, Red lists (national)) and international (Habitat Directive, Natura 2000, Bird Directive, Red lists (international)) policies. The policies have a legal status, except for some of the national policies (e.g. Ecological Main Structure, Red lists).

The target of the policies is protection of general biodiversity, habitats, habitats of specific species and species (both individuals of the species and their populations). All these policies aim at maintaining a favourable conservation status of their objectives. They usually try to achieve this by habitat protection (except in the Flora and Fauna act). The international policies state that no activities are acceptable which result in significant negative impact on the habitats or species. Pollutants may be one of the factors threatening the favourable status. Only in the Habitat Directive this aspect is specifically mentioned. Amongst others, population models are used to assess whether populations of species are threatened as a consequence of contamination.

#### **2.4.3 EU-Water Framework Directive**

The EU-Water Framework Directive (WFD) provides a framework for the protection of surface water, groundwater and coastal waters. The WFD describes which environmental targets should be reached and how and when these targets should be achieved using an integrated management at the river basin level. River basins are divided in smaller homogeneous units called water bodies. Upon implementation of the WFD, both chemical and ecological quality criteria will be set for each water body in the EU. The WFD prescribes a monitoring and reporting system from the local level to the community level. It describes how other existing (e.g. on risk reduction of chemicals, emission controls, bird and habitat directive) and future (groundwater) Directives and international agreements (e.g. the OSPAR agreement) are integrated or replaced to achieve the common WFD targets. River management plans are required that include pollution reduction plans and other measures that that will lead to a good chemical and ecological status or potential. Reports on the progress of the implementation of measures and of monitoring to assess the effects are mandatory.

The implementation of the WFD has an influence on most of the existing national policies and regulations on water quality. Important changes with respect to risks associated with toxicants are:

- the obligation for water managers to meet quality criteria in a fixed timeframe

- the introduction of ecological quality criteria
- abolishing chemical sediment quality criteria

Various exposure and effect models play a role in the context of the implementation of the WFD.

## 2.5 Protection targets and specific environmental policies

In this paragraph, some specific protection targets and specific environmental policies are outlined, according to the following sections: (1) a section introducing the issues of relevance, (2) a set of typical questions posed by policy, (3) a short overview of some models that are used.

### 2.5.1 Soil protection, sanitation and use specific criteria (BGWs)

#### *Issues*

The protection target for the compartment soil is clean soil, as defined by reaching the Target Value for all compounds. In the Netherlands, prevention of soil pollution is based on the Soil Protection Act, which came into force in 1987. To control soil pollution, instruments that can be used are the ALARA principle (As Low as Reasonably Achievable) and the use of best available techniques (BAT). The Act states that emissions and the resulting soil pollution can be tolerated so long as the soil quality does not decline (stand-still principle) and that the so-called ‘multifunctionality’ of the soil is not endangered. It is assumed that this encompasses a sustainable and autonomic functioning of the soil as provided by soil processes and soil biota.

For the implementation of this policy, so-called *Target Values* (TV) or criteria related to target values are used. As long as the concentrations of pollutants in soil remain below the target values, the soil is considered *multifunctional*, i.e. fit for any land use, bearing in mind any limitations due to the natural composition of the soil.

Regarding toxic compounds, many sites are exposed beyond the *Intervention Value* (IV). This is interpreted as a concentration level due to which sanitation is (in principle) warranted and for which a sanitation urgency and sanitation targets are to be established (VROM and Van Hall Instituut, 2000). However, reaching this situation would require a major policy effort, that will take various decades of sanitation activities (Kernteam Landsdekkend Beeld 2004) and a load of money. Currently, the policies are being changed, whereby more emphasis is put on site-specific risk levels rather than on mere exceedance of quality criteria *per se*.

Soil-use specific Remediation Objectives (SRO, or in Dutch “Bodem Gebruiks Waarden”, BGWs) have been developed as curative instrument (Lijzen et al., 1999). These SROs (BGWs) have the goal of creating a post-remediation situation in which the human and environmental risks, given a local soil use, are reduced to an acceptable level for that use. SROs indicate acceptable pollutant levels of the topsoil given a specific soil use. Four classes of soil use are distinguished: I. residential and recreational green areas; II. non-recreational green areas; III. built-up and paved areas; IV. agricultural- and nature areas. Of these four classes, the protection of ecological aspects is most important in class IV. In general, nature areas impose the strictest demands on basic ecological quality, since in these areas the presence of sensitive species such as target species (protected species) must be possible. In agricultural areas the ecological quality also has a high priority (e.g. importance of meadow systems for protected farmland birds). Next to these criteria, a basic approach has been

developed to address local effects of soil pollution on ecological quality (Rutgers et al., 2000 (in Dutch)).

Many soils in the Netherlands are polluted with a mixture of toxicants. Of these, a few hundreds of thousands are classified as being “highly polluted” on the basis of soil quality criteria. These sites are also located in agricultural and nature areas. More than 100.000 ha of agricultural land is considered contaminated with mostly heavy metals and part of the nature areas managed by conservation organisations are “highly polluted” (Van der Waarde et al., 2003). Although the sites are classified as “highly polluted” according to the current classification system, it remains unclear whether and in how far local ecosystems at such sites function sub-optimally as a consequence of pollution.

### *Questions*

Soil-use specific questions can be raised such as:

1. Are polluted areas still suitable for the soil-use function “nature”?
2. Does soil pollution negatively influence the viability of a Red List species like the godwit in agricultural areas?
3. What is the local risk of the mixture of compounds  $x_1 - x_n$  at site Y with soil conditions Z?
4. What is the general risk of spreading (slightly) contaminated sediments from ditches in the rural areas on adjacent soil?
5. And what is the specific risk of doing this on location x for the local nature development into the target nature type (e.g., flower-rich ditch borders, or the godwit population) within the general soil use category “nature”?

In the case of soil and soil protection, it should be noted that the evaluation of soil quality is currently changing considerably, as a consequence of the apparent magnitude of the problem of soil contamination. An array of activities is currently being undertaken in both the policy and the scientific arena, so as to more effectively solve the policy problems. This process was triggered by the publication of the so-called Policy Document on Soil (In Dutch: “Beleidsbrief Bodem”) by the Dutch government (VROM, 2003). According to this Policy Document, various changes are to be implemented, for example as a consequence of the notion that “more risks imply more management”. This calls, amongst others, for an improved set of site-specific risk assessment approaches, to enable local quantification of risks, as being dependent on the local mixture, the local soil type and the local soil use. This process has as yet not ended and it is thus unclear how to evaluate the models that might be used.

### *Models*

An array of models is used in soil assessments, amongst which exposure and effects models. Some examples are given, in addition to the models that were described above and that were used to derive the generic quality criteria.

A procedure is in operation to allow local stakeholders to determine sanitation need and urgency in cases where the Intervention Value is exceeded (VROM and Van Hall Instituut, 2000). In this procedure, the level of local risk as induced by the local mixture is determined in gross categories. Exposure and effect models are used, to address the site-specific situation rather than exceedance of generic risk limits (the IV). Thereby, not only the site-specific risk levels are taken into account, but also the volume of contaminated soil and groundwater.

A procedure is being developed for the Integrated Risk Assessment of sediment deposition on land. The sediment-soil system is described in a so-called systems approach and the fate of all compounds in this system is determined using exposure models. Thereafter, risks for soil organisms are determined using the SSD model. Eventually, the deposition of sediment on land can be judged by comparing the locally predicted Environmental Concentrations to the quality criteria and/or by the principle of stand still and /or by comparing the local risk levels that are reached to the originally defined protection target. The latter is, of course, the so-called 95% protection level, as introduced above (at the HC5, 95% of the species is protected against adverse effects of exposure, in this case: exposure to mixtures). The procedure that is being developed is currently awaiting inputs in the format of policy choices that need be made in the framework of the implementation trajectory that followed the publication of the abovementioned Soil Policy Document.

Since sanitation to the level of the TV is often not feasible, neither technically nor for societal reasons, the sanitation should at least proceed to the level where risks for the current soil use are acceptable. This resulted in the derivation of Soil-use specific quality criteria (in Dutch: Bodem Gebruiks Waarden, BGWs). These BGWs identify the level of contamination that can be present whereby the contaminant does not impose unacceptable risk given the local soil use. For example, the BGW for a soil use with intensive probability of human exposure (harvest of home-grown groceries) is lower than for a soil use with limited probability of exposure (garden without home-grown edible products).

BONANZA (Kros et al., 2001b) is a decision support system developed to support decisions of nature managers on the use of former farmland which are polluted with nutrients and heavy metals. BONANZA combines geographical maps with modules on soil pollution, soil quality and ground water tables and assesses the risk of pollution for the vegetation, for herbivores and for species that feed on earthworms. In this system an ecotoxicity module is implemented that exists of a part that calculates the available fraction of heavy metals, makes statistical risk assessment (PAF, see section 4.2 for an explanation of this “ruler”) and deterministic risk assessments for secondary poisoning such kidney lesion (Ma et al. 2001b). Within the model two terrestrial food-chains (Bosveld et al., 2000)(Klok et al., 2005). The PODYRAS model is used to assess effects of lower food availability.

## 2.5.2 Side effects of pesticides

### *Issues*

Most regulatory documents that deal with pesticides (Plant Protection Products, PPPs) are based on policy goals that are ambiguous or difficult to define or measure. In the EU Uniform Principles (EU, 1997) it is amongst other things stated that:

- the influence of PPPs on the environment should not be unacceptable (comment: leaving room for interpretation of the degree of impact that is acceptable)
- Member States shall ensure that use of PPPs does not have any long-term repercussions for the abundance and diversity of non-target species (comment: suggesting that shorter-term impacts followed by recovery are acceptable)
- No authorisation shall be granted ..... unless it is scientifically demonstrated that under field conditions there is no unacceptable effect on the environment (including impact on non-target species) (comment: suggesting a science-based risk assessment with a tiered approach).

The “unless” clauses formulated within the context of the Uniform Principles (Directive 91/414/EEC) tend towards the application of the Community Recovery Principle, at least for



the multifunctional ecosystems in and adjacent to the sites of application (e.g. drainage ditches). The Community Recovery Principle presupposes that an ecosystem can absorb and endure a certain amount of pollution because of ecological recovery processes. The stressor should be limited to an intensity or concentration that causes short-term impacts only on the most sensitive populations. From a scientific point of view, periodically occurring declines in population densities can be considered a normal phenomenon in ecosystems, which is called resilience. Organisms have developed a large variety of strategies to survive and cope with temporally variable and unfavorable conditions such as desiccation, flooding, temperature shocks, shading, oxygen depletion, food limitations, toxins in food, as well as anthropogenic stressors (Ellis, 1989). In some cases, but certainly not all, the stress caused by a PPP may more or less resemble that of a natural stress factor. The use of the “normal operating range” of population densities and functional endpoints in specific ecosystems has been suggested as a baseline against which to assess pesticide-induced changes (Domsch et al., 1983). In other words, effects of PPPs of which the bioavailable fraction is restricted in space and time may in certain habitats be regarded as ecologically unimportant when they are of a smaller scale than changes caused by other natural or anthropogenic stresses (Brock, 2001).

### *Questions*

1. Are there side-effects of pesticides after spraying in real field conditions?
2. Can the side-effects of pesticides be reduced by choice of different application regimes, i.e., by reducing exposure of non-target habitats (local ditches bordering the sprayed field, non-sprayed field borders)
3. Can pesticide application regimes be optimized so as to reduce impacts, when exposure reduction measures themselves cannot be reduced more?
4. What happens upon spraying of tank mixtures, or after repeated application over time?
5. Is it likely that ditch ecosystems show (full) recovery after an impact?
6. What degree or time-span of impact is limiting full recovery?

### *Models*

Within Dutch pesticide registration, pesticide fate models are used to assess exposure in surface water and leaching to groundwater. Exposure in surface water is based on simulations with the TOXSWA model (acronym based on TOXic Substances in surface Water, see Adriaanse (1996)). TOXSWA simulates behaviour in surface water including convection with water, sorption to macrophytes, diffusion into sediment, sorption to sediment and degradation in water and sediment. The exposure assessment is based on calculations for a spring and an autumn scenario (not containing macrophytes). For both scenarios, spray drift is the only source of surface water exposure with pesticides.

Leaching to groundwater is assessed with the PEARL (Leistra et al. 2000a) and GeoPEARL models (acronym based on Pesticide Emission At Regional and Local scale, see Tiktak et al. (2003)). PEARL includes processes such as convection with water flow, sorption to solid phase in soil, degradation in soil and uptake by plants. GeoPEARL links PEARL to GIS databases on land use in the Netherlands and the Dutch soil map. Using this tool, calculations can be made for the intended area of use of the pesticide. In the first step of the assessment, calculations are made with PEARL and a single scenario (i.e. the Kremsmünster scenario developed for use at EU level). In the second step of the assessment, calculations are made with GeoPEARL.

On the effects side, the use of models is less developed. The Species Sensitivity Distribution concept (Posthuma et al., 2002b) is used in the effect assessment for the aquatic ecosystem, while applications for terrestrial, bird and mammal assessments are expected. This concept is used to calculate the HC5 (Hazardous Concentration 5%) from a collection of relevant laboratory toxicity data, which is estimated to be protective for field communities (Maltby et al., 2005). Other models like the ecosystem model PERPEST (Van den Brink et al., 2002c), the recovery model HERBEST (Van den Brink and Kuyper, 2001) and metapopulation models (Spromberg et al., 1998) are not routinely used, but hold great promise for the future.

### 2.5.3 Nature policies and global backgrounds

For many decades there has been a substantial loss of biological diversity worldwide and in Europe due to human activities (pollution, deforestation, etc.). Biodiversity is seen as one of the key indicators of success, to quest for the sustainable use of natural resources. The Convention on Biological Diversity (CBD) was signed by the European Community and all the Member States at the United Nations Conference on Environment and Development in Rio de Janeiro from 3 to 14 June 1992. This EU-decision approves the Convention on behalf of the European Community. The United Nations Environment Program (UNEP) estimates that up to 24% of species belonging to groups such as butterflies, birds and mammals have completely disappeared from the territory of certain European countries. For this reason the Convention contains 59 objectives for conserving and enhancing species and habitats as well as promoting public awareness and contributing to international conservation efforts. A cross-sector Steering Group was set up to progress four main areas: key species and habitats, access to biodiversity databases, public awareness and involvement, monitoring systems.

### 2.5.4 Policies on area protection

#### *Issues*

At the EU-level, the *Habitats directive* (Directive 92/43/EEC) is aimed at protecting habitats and at protecting a set of species that is listed in its Annex I and II. Species in these Annex lists are mammals, reptiles, amphibians, fish, arthropods, mollusks and plants. Birds are addressed in the *Birds directive*.

Conservation of these species is by protection of their habitats. The Directive (Article 1) states that measures should be taken required to maintain or restore the natural habitat of the populations of species of wild flora and fauna at a favorable status. This means for species that (point i of Article 1) population dynamics data on the species concerned must indicate that it is maintaining itself on a long-term basis as a viable component of its natural habitat. For the species listed in this Annex II, Special Areas of Conservation (SAC) must be designated and these constitute the so-called “Natura 2000” sites. The protection of the SAC sites is described in Article 6. Article 6(1) makes provisions for the establishment of the necessary conservation measures and is focused on positive and proactive interventions. Article 6(2) makes provisions for avoidance of habitat deterioration and significant species disturbance. Its emphasis is therefore preventive.

As an example for the United Kingdom, a Steering Group report, published in 1995, contains Species Action Plans (SAPs) for a “short list” of 116 of the UK's most threatened animals and plants. It recommended the drawing up of a further 286 plans for “middle list” species. These lists are now simply referred to as the “priority species”. Out of 45 Habitat Action Plans (HAPs) for the UK's most threatened and important habitats, 14 are included in the

Steering Group Report. The remaining SAPs and HAPs were published in the Tranche 2 Action Plan series in 1998-1999.

Furthermore, article 6(3) states that “any plan or project not directly connected with or necessary to the management of the site but likely to have a significant effect thereon shall be subject to appropriate assessment of its implications for the site in view of the site's conservation objectives”. Only after having ascertained that it will not adversely affect the integrity of the site concerned such a plan may be considered.

For the Netherlands, an array of policy actions were already set in operation, or they were adapted from earlier ones and new ones are adopted. The new *Nature Conservancy Act* succeeds the one which came into force in 1967. In the old version of the act, nature areas were re-established and maintained and plant and animal species protected. The 1967 Act, however, was not in compliance with the international obligations of the Birds and Habitats Directives. The new version of the Act came partly in force in 1998 (the Flora and Fauna Act). This Act will protect areas in compliance with international obligations. This Act is foreseen for 2005. As long as this Act is not in force, Article 6 of the Habitats Directive is included in the Flora and Fauna Act and areas are protected in the “Natura 2000” sites. At these sites, protection is attained by conservation measures which correspond to the ecological requirements of the natural habitats in these sites, measures to counteract deterioration of natural habitats and habitats of species as well as disturbance of the species for which the areas have been designed. New activities at these areas are only acceptable if they have no significant negative implications for the habitats or species.

The *National Ecological Network* was introduced in 1990 by the ministry of LNV. This network connects nature areas such that risk of extinction of plants and animals as a result of fragmentation is reduced, while nature areas keep their value by not being too small. Among others, “Natura 2000 sites”, reserves and agricultural areas can be part of the “Ecological Main Structure” (EMS). The design of the EMS is mainly based on spatial aspects (area size and connectivity) of the habitats, while quality aspects such as soil pollution play a minor role. The process of designating the EMS was initially covered by land development projects and later by an area-specific policy. In selecting the designated areas, account was taken as far as possible of current and potential natural features (nature values). The protection of the EMS has not a legal status; it has a regulatory status.

Policies for area protection have ecosystems, habitats and species (individual and population level) as targets. Most measures to improve the areas are directed at improving habitats. Where does pollution *specifically* conflict with policies for area protection?

- Flora and Fauna Act. Article 9 states that it is prohibited to kill or injure animals and Article 11 states that it is prohibited to disturb and destroy their habitats.
- All the SAC sites which are included as parts of the National Ecological Network are under legal protection as set out in the Birds and Habits Directive. Other EMS sites are only protected by spatial planning. This implies that activities are only permitted within the site if they do not change the characteristics of the site.
- The Dutch policies for the Habitats Directive states that habitats and species must be kept in favorable status, which implies for species populations that they can maintain themselves on a long term basis. Article 6 clearly states that any activity which has a

significant effect on the status of a habitat of species population should be avoided. This includes impacts of pollutants.

In conclusion, soil pollution may conflict with these policies and both prohibitive and curative measures may be taken. In the prohibitive sense: it is not allowed to start activities that pollute habitats of protected species or that endanger their survival nor their population viability. In the curative sense, sometimes, measures need be taken if habitats are deteriorated in such a way that the policy targets might be affected.

### *Questions*

Policy questions related to these subjects are, for example:

1. General: Given protected areas in which contaminations have been observed, what is the relative vulnerability of target species compared to the generic species pool?
2. *Ibid.*, how are vulnerabilities amongst target species related? Is one (by far) more vulnerable than the other? Can this be explained by one or more typical biological features in the biology of the species?
3. Specific: Does cadmium and copper pollution of a soil result in lower population viability of the badger in a fragmented habitat as compared to a non-fragmented habitat?
4. Does pollution have a negative impact on species in a highly dynamic environment such as a river floodplain?

### *Models*

For the policies directed at area protection, a suit of models can be applied. The choice of a model depends on the specific question and available ecological knowledge on the specific system. The available models range from qualitative expert knowledge based information models, quantitative statistical risk models to population dynamic models. As with species policies, both risk and effect based models can be of importance. Models applicable for prohibitive policies should be able to assess the risk of pollutants on species and habitats, especially on their status. For species this assessment target is formulated as their long term viability. These models should be either directed at the species population level of the habitat level. For curative policies assessment of the risk of soil pollution in a protected area can be assessed starting with generic models (such as SSDs) and being fine-tuned with species models (such as matrix models). The more specific questions can be addressed by using an expert judgment model. An example is a sensitivity analyses based on ecology and toxicology (Faber et al., 2004). Combined effect assessment of the risk of secondary poisoning and food shortage in combination with fragmentation can be done with the model PODYRAS (Klok et al., 2000). The impact of flooding on population viability of earthworms and the consequences for predators can be determined using the model PODYRAS (Klok et al., 2005)

## **2.5.5 Policies on species protection**

### *Issues*

At the EU-level the *Birds- and Habitats Directives* provide a protection framework for birds and areas. The Birds Directive (Regulation 79/409/EEG) came in act in 1979. This Directive relates to the conservation of all species of naturally occurring birds in the wild state in the European territory. It covers the protection, management and control of these species and lays down rules for their exploitation. Measures are directed at keeping populations viable. The conservation of all bird species is established by the preservation, maintenance and re-establishment of their biotopes and habitats and includes creation of protected areas, upkeep

and management in accordance with the ecological needs of habitats inside and outside the protected zones, re-establishment of destroyed biotopes and creation of biotopes. The species mentioned in Annex I of the Directive are subject to special conservation measures concerning their habitat, in order to ensure their survival and reproduction in their area of distribution. For these species, trends and variation in population levels are taken into account as background for evaluation. Special notice is made of pollution in Article 4 which states that Member States shall take appropriate steps to avoid pollution or deterioration of habitats or any disturbances affecting the birds, in so far as these would be significant having regard to the objectives of this Article. Outside these protection areas, Member States shall also attempt to avoid pollution or deterioration of habitats.

*The Flora and Fauna Act* (In Dutch “*Flora- en faunawet*”) came into force in 2001. The Act incorporates the old Hunting and Birds Act (In Dutch “*Jacht- en Vogelwet*”) and also parts of the Nature Conservancy Act pertaining to protection of species. This act provides wild species of flora and fauna with legal protection. Article 9 states that it is prohibited to kill or injure animals and Article 11 states that it is prohibited to disturb and destroy their habitats.

The Flora and Fauna Act provides passive protection (by law) and is therefore a reactive instrument. Next to this reactive protection instrument the ministry of LNV also developed *instruments* for active protection of species which strive for increase of quality of habitats and survival probabilities for species. Instruments are The Long-range Implementation Program for Species Policy (In Dutch “*Meerjarenprogramma Uitvoering Soortenbeleid*”), species protection plans and red lists. The Long-range Implementation Program for Species Policy was introduced in 2000. This program is directed at development and implementation of species protection plans. Species are placed on a Red List when they are endangered, i.e. rare or declining in number. A restricted number of species, most of them endangered, are covered by species protection plans, which specify the measures needed to ensure their survival. Next to species protection plans red lists were developed on the initiative of the IUCN.

*Red Lists* indicate species whose survival is threatened. These lists are one of the outcomes of the Bern Convention, which was ratified by the Netherlands in 1982. Red lists were renewed and extended in 2004. Traditionally Red lists were especially for birds and mammals and some other taxonomic groups. The renewed lists also include plants and insect species. Threatened species are only included in the Red lists if they breed in the Netherlands. Red lists species do not automatically enjoy legal protection, for this they must be included in the Flora and Faun Act, but the law stipulates that the government must make efforts to protect these species and promote research to that end.

International *Red lists* are based on the Criteria for Status defined by the World Conservation Union (IUCN). Criteria for the status are Critically Endangered, Endangered and Vulnerable. They are strongly based on the population viability of the species, population size reduction and population growth rate. Protection therefore is at the population level.

*Species protection plans.* Each year since its introduction, a total of five plans have been drafted in the framework of the Long-range Implementation Program for Species Policy. The first species protection plan dates from 1984. Plans have been developed for 21 species, most of it mammals (e.g. badger) and birds (e.g. barn owl). Species protection plans indicate which extra measures are needed to protect endangered species in the Netherlands. These measures may concern improving the quality of the environment (a habitat approach, which also is

beneficial to other species), or the definition of specific species directed management measures. The habitat approach is given priority in a number of species protection plans, for example in the one pertaining to marshland birds.

Species are obviously the targets for policies on species protection. Restrictive policies such as the Flora and Fauna law prohibit activities that may destruct habitat of species, disturb species or directly act on them (killing). Other policies such as the Bird Directive are both restrictive and active (curative) by on the one hand prohibiting activities that threaten species or their habitat and employ curative measures to increase the population viability of the species. Species protection plans are curative in that they strive for improvement of the habitat of protected species. Most measures to improve the viability of the species are directed at improving their habitats or have specific objectives such as increasing the number of nest sites (e.g. species protection plan on the barn owl).

When does soil pollution conflict with policies for species protection? In the prohibitive sense, general activities that endanger the protected species or their habitat are restricted. Bringing pollutants in protected areas or inflicting direct risk at protected species is therefore prohibited. Only the Bird Directive explicitly states in Article 4 sub 3 that Member states shall take appropriate steps to avoid pollution or deterioration of habitats, also outside protected areas they shall strive to avoid pollution. In the curative sense, active protection of species may warrant remedial action (species protection plans, Red Lists, Bird Directive). Species may have their habitats in polluted environments. If soil pollution threatens their viability, curative measures may be taken to improve the habitat.

### Questions

Possible questions are:

1. Does soil pollution reduce population viability of a target species?
2. What is the relative risk of soil pollution compared to other environmental stress factors such as inundation frequency in floodplain ecosystems?
3. Is the population viability of the godwit reduced in the area of the *Ronde Venen* compared to the non polluted *Zeevang* area?

### Models

Models applicable for species protection policies can range from qualitative expert-knowledge based information models, to quantitative food-chain models and population-dynamic models. Both risk- and effect-based models can be of importance. Risk-based models can be applied for restrictive policies to assess e.g. the impact of activities which bring pollutants in the environment of protected species on these species. Effect-based models can be applied to assess the actual impact of soil pollution present in their environment. These models can be directed at the individual level, using e.g. bio-concentration factors or the time to reach critical values in organs, e.g., (Klok, 2000)), or at the population level (e.g. (Klok and De Roos, 1998)).

Although not always explicitly stated (e.g. Flora and Fauna Act) species protection is generally at the population level. Restrictive policies indicate that viability may not be endangered by activities, whereas active protection policies state that protection measures should be increase population viability of endangered species. This means that models applied to interpret the risk or effect of soil pollution should be directed at the population level. Such models are not available for all systems, nor can be constructed given the absence of basic life-history data of species (e.g. survival and reproduction). Therefore, if absent,

other models that require less data input such as bio-accumulation models can be applied to assess the risk of secondary poisoning on the basis of food choice, food intake rate and concentrations of pollutants in food. These models, however, cannot indicate the impact of soil pollution on population viability. When also no data on food choice and intake rate are available, expert judgement may give qualitative insight in risk levels.

Examples of models applicable for the specific questions stated above are Simple matrix models, from which the methodology has been developed by Caswell (2001). The methodology is applied for some species (e.g. Crouse et al., 1987; Doak et al., 1994). More specific questions on the relative risk of soil pollution compared to inundation frequency on population viability of earthworms (as important food source for target species) has been explored with the earthworm model PODYRAS (Klok et al., 2005). Another example is a case study in which life-history data at a polluted and reference site are assembled for the godwit and these data will be used to parameterise a population model for this species (Roodbergen et al., in prep)

## 2.5.6 Water quality management

### *Issues*

The Water Framework Directive (WFD) combines two approaches at the same time. Waterbodies have to comply with a good chemical status and at the same time with a good ecological status or potential. For each waterbody, monitoring of the chemical and ecological quality is required.

*Chemical status.* The EC identifies priority substances and sets of quality criteria for these substances. This is a limited set of compounds, currently comprising 33 substances or groups of substances, for which quality criteria apply to all waters. In addition, there are guidelines to identify additional relevant substances for each river basin. Criteria for these substances are to be set at a national level and tuned with other countries sharing the riverbasin. When the chemical quality criteria are not met, the sources should be identified and actions be taken to reduce emissions from point and diffuse sources, which may include sediments.

*Ecological status.* Ecological quality criteria are derived for specific groups of organisms: fish, benthic invertebrates, phytoplankton and macrophytes or phytobenthos. Derivation of ecological quality criteria is done on a regional scale and harmonised in an intercalibration procedure. No final criteria have been set yet.

When the ecological criteria are not met, an investigation of causes is required (investigative monitoring). These causes may include chemical pressures. Models like OMEGA123 may help identify and quantify the role of chemical pressure. For a further example: see Appendix 1, in which an OMEGA-related model (IQtox) is used together with ecological modelling, to identify magnitudes of local impacts and probable causes.

Organisms higher up in the foodchain that may be susceptible to secondary poisoning are not included in the standard ecological quality criteria of the WFD. However, in special protected areas under the Bird and Habitat Directive, these may be among the target species and should be protected. The effects of secondary poisoning to these organisms could be investigated using OMEGA45.

*Issues: Soil protection act*

A revision of the soil protection act (In Dutch: “*Wet Bodembescherming*”, *Wbb*) introducing new remediation targets and criteria will be published in 2005. Remediation targets for terrestrial will be land-use dependent. The WFD however does not allow differentiation of criteria according to use. Remediation target for sediments will therefore be the good chemical and ecological status or potential of the WFD. Presently it is not likely that there will be criteria for sediment quality under the WFD. Sediments will be regarded as sink and source of compounds that may affect the water quality for which criteria are set. Sediment quality is also evaluated for the effects on ecological quality parameters (e.g. benthic community composition). Both models, bioassays and assessment of field-effects may be used to reveal the relation between sediment quality and ecological quality parameters. The most recent proposals include the use of msPAF calculated with OMEGA123 as method to establish reaching the remediation criterium.

*Issues: Disposal of dredged sediment*

Dredging of accumulated sediment is necessary to maintain the functions of waterways for water quantity regulation and shipping. Large volumes of sediment are involved which should preferably be spread on the land. Due to the presence of contaminants in the sediment and stringent criteria to prevent soil pollution, the spreading of this material is often not allowed. As a result maintenance of waterways is delayed. A prototype of the model *IRAsed* has recently been developed to provide a means to assess the risk associated with spreading of contaminated sediment. Depending on the regulatory decision to be taken on this approach, it is considered likely that its implementation will reduce the volume of sediment that can not be spread on land, while not introducing unacceptable risks for terrestrial organisms (man, ecosystems, agriculture) locally.

*Questions:*

1. Does the contribution of contaminants explain the low quality of the ecological conditions of an ecosystem?
2. Which emissions are allowed in a certain water body?
3. Emission management plans need to be in place. Which compounds are (most) important for being subject to regulation (highest impact)? What is the relative priority amongst compounds for regulatory action?
4. Which compounds should be monitored to help guaranteeing “good ecological quality”?
5. What is the consequence for the aquatic environment when a garbage dump site starts leaking towards surface waters in the surroundings?

*For the sediments and soil, questions are:*

1. To what extent can toxic pressures explain non-compliance of waterbodies with ecological quality criteria?
2. Many waterbodies in the Netherlands are designated artificial or heavily modified waterbodies. These waters do not necessarily need to comply with a good ecological status, but are required to provide a good ecological potential. Models could help decide whether toxic pressures limit the ecological potential.
3. Are targets of special protected areas of the WFD, e.g. those assigned by the Bird and Habitat Directive, at risk from contaminants.
4. To increase the water storage and discharge capacity of the river bed, (contaminated) sediments of river forelands are partially removed. What are the remaining risks for the ecosystem after lowering of river foreland?



5. What are the risks to the receiving soils of spreading dredged sediments on land? Several models are used to aid assessment of sediment and water quality. An exposure and effect model will be used to evaluate the suitability of dredged sediment for disposal on land (land-use oriented).

### *Models*

In general, ecotoxicological models can help to identify the causes of impacts. In particular, the EU-project Rebecca designed to deliver relationships between chemical pressures and ecological responses, has chosen OMEGA as the principal model for toxicants (<http://www.environment.fi/syke/rebecca>).

The OMEGA model has been used in various cases. For example by:

1. setting priorities of chemicals to be reduced in regional emission management plans by determining the substances that affect the ecosystem most
2. by weighing the pro's and con's of nature development in contaminated floodplains
3. by identifying the most dangerous chemicals and the most vulnerable species to be monitored in regional chemical analysis and ecotoxicity assay programs and
4. by estimating possible consequences of leaking waste sites for the nearby ecosystems.

## **2.6 Reflection on Protection Targets and Models**

Models are used in the pertinent policies to cover and help solving the risk management problems. The models are linked by underlying modelling principles and protection targets. The following key protection target has played a role in the derivation of the solutions to all the separate policy problems:

A fundamental strive to protect ecosystems (aquatic, terrestrial, sediment) from structural damage and to formulate protective and curative policies to reach this target by source- and effect oriented tracks. Similarly, a fundamental strive to protect ecosystem from functional damage.

As said before, models may be used to perform risk assessments in the evaluation of substances for permissibility purposes. For this purpose, they guide the definition of protection targets in general terms (protection of ecosystems) as well as in terms of the protection of certain species or processes within ecosystems. Additionally, these models can be applied to perform calculations for exposure and effect scenarios to estimate consequences of human interference in advance. These model calculations also aid decision-making procedures in the comparison of scenarios or designs. Models that estimate effects of sludge application on a certain area in terms of loss of species or ecological functions and models that determine the urgency and targets of soil restorations may be regarded as illustrations of this type of application of ecotoxicological models. These models can also serve in the determination whether or not an area should be acquired for a certain future purpose and subsequently, they guide nature redesign and development projects. Regarding these site-specific assessments, ecotoxicological models can also be applied to establish a spatially differentiated set of environmental quality standards. Furthermore, they may be applied to support environmental policy reports including the Environmental Balances, Environmental Outlooks and Nature Balances to develop system-oriented nature (conservation) policies and to determine the causal contribution of the presence of a substance to the incidence of a certain species in an area.

A summary of some selected policy problems is provided in Table 1.

*Table 1. A selection of environmental problems encountered by the 3 different ministries given their specific responsibilities in policy making*

<b>Ministry</b>	<b>Policy target</b>
VROM	<u>Preventive policy: generic</u> Setting Environmental Quality Criteria, e.g., Target Value Regulation of newly developed compounds (e.g. Pesticides, “New Substances”)
	<u>Curative action policies</u> Setting and use of Intervention Values and assessment protocols like Sanitation Urgency System
	<u>Monitoring</u> National or regional trends analyses, e.g. for toxic stress, to support emission reduction decision Specific, target compound / compound group trends analyses, e.g., for pesticides
LNV	<u>Preventive policy: generic Nature policies</u>  <i>National: Flora and Fauna Act (Flora en Fauna wet)</i>  <u>Policies for Species protection: specific</u> Species protection policies (Soortbeschermingsplannen); National Red List (nationale Rode Lijst soorten), International: Birds directive (79/409/EEG); Red list  <u>Policies to protect biodiversity in areas</u>  National: Nature Conservancy Act (Natuurbeschermingswet); Ecological Main Structure (EMS) International Habitats Directive (92/43/EEG); Natura 2000  <u>Policies to avoid undesired side-effects of pesticide use</u> Pesticide assessment protocols in NL and EU
V&W	<u>Water management policies</u> Good chemical status, setting EQCs for catchments Good ecological status, setting biological references for catchments Monitoring, identifying impacts and causes of impacts Managing sediment quality and reaching sediment quality criteria Managing sediment deposition on land

### 3. An integrated toolbox of ecotoxicological models

#### 3.1 General

Chapter 2 has formulated a set of protection targets and subsequently (despite different policy targets) the underlying models used to address those protection targets. These models consist of a relatively small set of basic models. Thus, ecotoxicological models find their application in a wide range of environmental problems. Most of these policy problems concern the estimation of the effects on the environment of human interference. However, many ecotoxicological models are applied to estimate hazards, which can be described as the chance that an effect may occur, leaving aside the extent of the effects. To overcome this dissimilarity, the endpoints of ecotoxicological models need to be tailored to endpoints in environmental policy design to improve their application.

The aim of this Chapter is to order models according to their first principles (i.e., what is the scientific basis for the model and the scientific approach used) and further to order them in an array of practicality for daily use (“tiering”). The viewpoint that is taken is that of “creating a toolbox”, so that models and approaches can eventually be easily linked to the policy problem to be addressed, whereby it is clear “what tool is for which problem” – and when not to use the tool. Evidently, some models do not fit to some problems, like SSDs not to predicting population viability of certain species. These limitations will evidently be part of the toolbox concept and the options of tiering therein.

#### 3.2 The toolbox concept

What is – in general – a toolbox?

*A toolbox is defined as a multi-tool instrument that enables a specific application of risk assessment, e.g. the derivation of human health based soil quality standards, or the assessment of the site-specific risks for the ecosystem. The application is as standardized as possible and as flexible as necessary. A toolbox can be a manual, a decision support system, or a computer program*

(taken from a discussion document of Swartjes, for RIVM-project “Risks in relation to soil quality”, where one also strives towards a toolbox for soil-oriented modelling).

The Toolbox will in part consist of models, for another part of other risk and effect assessment protocols, like an assessment based on a Triad of techniques. As to the idea of the toolbox, the first analysis is to identify exactly what the policy problem is. Thereafter, one can decide on modelling (or another technique) and on which model to use: “If the problem is a nail, use a hammer”. The toolbox can, however, not be used without guidance or limitations. Some approaches or models may not be suited for a certain purpose, for example, because they pertain to a different scale of effects, or because they have large data requirements as compared to the assessment problem. These are key notions for establishing a toolbox system that is tiered.

### 3.3 Tiered approaches to link protection targets to models

#### 3.3.1 The motives for tiering

Any ecological risk assessment that would *only* be driven by science would likely show application of the best of available methods, resulting in detailed and more or less uniform outcomes across different risk assessors. However, choosing a science-driven approach would result in costly assessments, even for the smallest risk problem. Combining pragmatism and science in risk assessment, one can understand the development of tiered systems, with simple, fast and cheap approaches in lower tiers and increasing complexity, time-consuming and costly approaches at higher tiers. The higher the tier, the more risk assessment problem are specified and the clearer the protection targets are defined by the stakeholders. The more specific the protection target or the system under investigation, the more the models that are applied should be tailored to the specific problem. As an example, Figure 3 shows how the outcomes of a tiered system responds to the change of methods across two tiers.

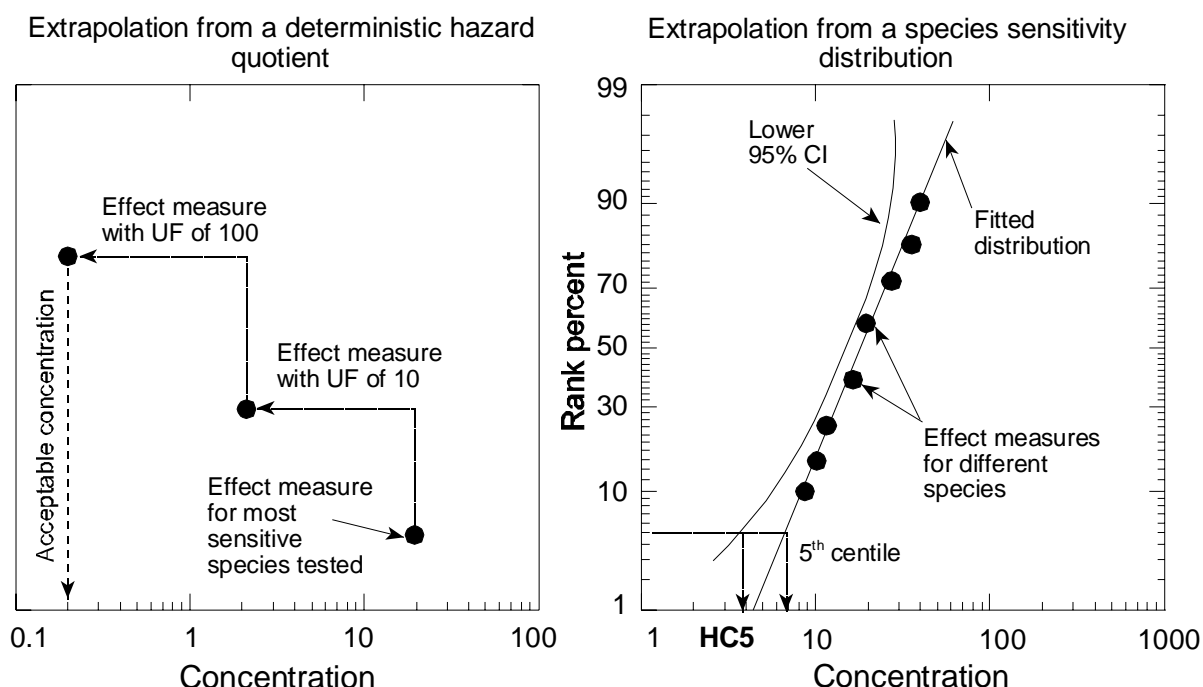


Figure 3. How tiering affects the outcome of an assessment, in this case the derivation of a generic EQC.

In the left part, the data from the most sensitive species are chosen and uncertainty in the assessment is taken into account by division of this value by 10 or 100, dependent on the number of data; the criterion value is either approximately 2 or approximately 0.2 as a result. Right: all data are used, a statistical extrapolation is used and the HC5 appears to be approx. 5.

A tiered system can be defined when protection targets can be refined in a stepwise way. For example, *general* environmental protection asks for the derivation of generic Target Values, whereby a simple “generic” use of the model of Species Sensitivity Distributions is warranted. Data for all species for which toxicity data of sufficient technical quality are available are used to derive SSD, accordingly to derive the generic TV. The TV is assumed to be sufficiently protective in all possible conditions.

However, assessing local risks for a specifically operating compound, such as a pesticide sprayed in a certain amount over a certain area, could ask for a higher-tier approach. To explain, the question is: should attention be paid to the sensitive species groups (those that possess the molecular receptor for that compound) apart from attention for less sensitive groups (non-target species). Should the assessment make clear that certain species groups in the sprayed area are affected more than others?

### 3.3.2 The principle of tiering in risk assessments

Tiered approaches solve problems in practical assessments by an efficient use of resources. Figure 4 illustrates the tiers in a risk assessment processes, showing the refinement in the process with acquisition of additional data. Simple approaches are, by definition, of low accuracy and are therefore designed to be conservative. More realistic approaches (higher tiers) require more data, are designed to have higher accuracy and uncertainty in the final outcome can be quantified. Quantification of uncertainty is, at least in the scientists' view, as necessary for informed decision making processes as are the assessment outcomes themselves. For risk managers, the uncertainty may be difficult to understand and handle and they may ask not to be confronted with the uncertainty itself, but only to the scientists' impression as to incorporate the uncertainty in the conclusions themselves.

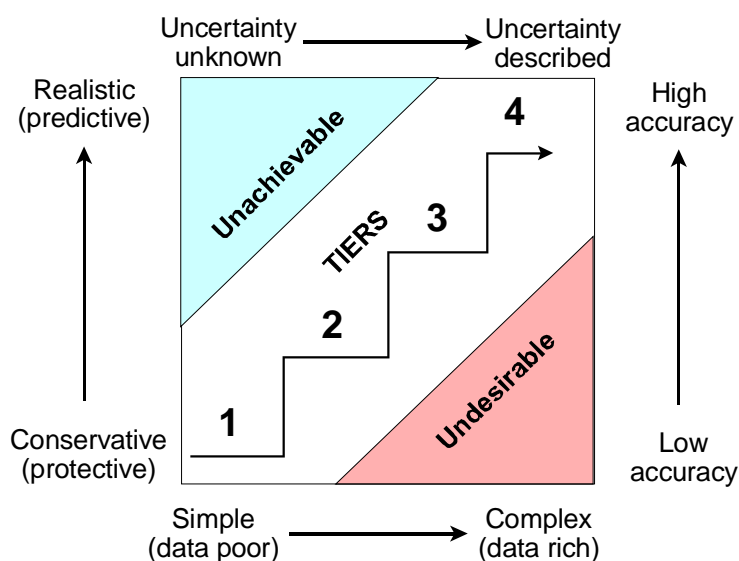


Figure 4: Tiers in risk assessment processes, after Solomon et al. (Solomon et al., in press)

A key requisite for proper function of a tiered system is that lower tier approaches are more conservative. This means that they should over-estimate risks to a certain extent. If, in lower tiers, risks appear acceptable, one can stop the procedure. Further, a requisite is that higher tier assessment results have more detailed information and therefore are more accurate. Therefore, they should over-estimate risks to a lesser extent than lower tiers. If the latter would not be the case, one would wrongly conclude to stop the assessment in a lower tier (false negative), while better methods would indicate serious risks. That is clearly undesirable.

### 3.3.3 Guidance on tiering

With no *a priori* idea on how to design a tiered toolbox, the application of tiered approaches could easily end up in an array of different outcomes for one assessment problem, i.e.

depending on the assessor who executes the assessment. For instance, one assessor could effectively, cheaply and fast apply state-of-art, higher-tier methods, while another assessor would start at the lowest tier. Evidently, applying tiers without guidance can result in an adverse public perception on the quality and accuracy of the output of risk assessments.

To avoid this, tiered systems in ecological risk assessment should therefore be designed according to some general rules and guidance should be provided, regarding two major issues:

1. Science: the system is internally consistent, that is: lower tiers are indeed more simple in principles and result in more conservative output than higher tiers
2. Practice: the system consists of a set of methods so that one can tailor the assessment method to the problem to be solved, that is: method costs and complexity range from low to high

These issues form the combination of the science-driven and practice-driven views on tiering. Shortly, a book will be published on the use of extrapolation techniques in ecotoxicology, touching on the subject of tiering. This biook will contain a Chapter providing guidance in the use of models in a tiered system (Posthuma et al., in press).

For the composition of a Toolbox, systematic evaluation of both available scientific methods as well as their pragmatic usage is warranted. Next, experiences gained with the toolbox should be fed back to the toolbox-manager, to improve on the contents of the toolbox and the utility of its parts. The phase-2 SSEO-validation efforts are planned precisely for that aim of providing feedback on utility of models for addressing environmental problems.

### **3.3.4 Existing approaches are tiered**

Many of the existing approaches in practical risk assessment are implicitly based on the concept of tiering. Tiering has been introduced to make efficient use of resources in risk assessment: simple problems are addressed by simple, generic methods and only when needed, more complex methods are warranted.

However, only few initiatives have as yet been taken to develop a more systematic approach in designing tiered systems for risk assessment methods that are used for policy support. Such efforts should account both: definitions of protection targets (generic or specific), policy problems (generic and specific) and available scientific methods. This subject is addressed further in Posthuma et al. (in press).

## **3.4 Model types: from exposure to effects**

Current ecotoxicological risk assessment models can be classified according to the biological level at which they generate an answer. Many models were applied to assess the effect of a chemical on individual organisms, but these are poor estimators of effects of chemicals at field conditions, as they do not take into account the evident dynamic processes within ecosystems that may influence the extent of effects. However, the complexity of ecosystems is overwhelming and it is questionable if our scientific knowledge of these processes is sufficient to predict the nature and extent of the impact that chemicals may have. The assessment of toxic effects in the ecosystem implies exposure of a complex biological system, with a great variety of species and exposure routes.

Nevertheless, the demand to manage the risk of chemicals in ecosystems is apparent and ecotoxicological models are needed to assess risks beyond the individual level, that is: at the

population and ecosystem levels. The models that have been applied at this level may be separated in a group of models that applies statistical methods and a group that applies our current mechanistic knowledge. Although emphasis in the SSEO-program is on effect-oriented models, no risk assessment can do without a proper analysis of exposure. Hence, this Section starts with a description of exposure modeling. An overview of the models is given in Table 2 (page 73), where (along the vertical axis) the models are ordered according to target (exposure or effect analyses) and type (empirical, mechanistic, expert system). Note that the list of models runs into the dozens, as shown in a recent inventory of Pastorok et al. (2002).

### 3.4.1 Exposure models

Recently, De Zwart et al. (2004) have prepared an overview of exposure models, according to a tiered toolbox approach. In that paper, the authors reviewed the existing literature of models that are (or can be) applied in practice. In media and matrix evaluation, three general levels of complexity can be recognized. The most simple approach assumes that all toxicants are completely available to be taken up by the biota. In this case, no extrapolation is required. A slightly more complicated step in the extrapolation process requires the calculation of (bio)available fractions of toxicants. The highest level of complexity additionally includes the action of physiological processes to the expression of the results, since it is eventually the interaction between toxicant molecules and targets sites of actions within organisms that determine the magnitude of effects. To a large extent, not the *total* concentration in a compartment determines uptake, but that concentration in combination with the properties of the matrix and the properties of the toxicant determine the uptake of a toxicant by the biota and thus the consequential effects.

In general, a large difference can be observed between the methods available for calculating matrix interference with organic and inorganic toxicants. Organic compounds are considered to follow the rules of equilibrium partitioning between the large-molecule organic constituents of the matrix and the lipid content of the exposed organisms. A number of computer operated models are available for predicting equilibrium partitioning exposure. The required input for those models (partitioning coefficients or fugacities and proportions of partitioning compartments) are, in general, easily available. For inorganic toxicants, mainly heavy metals, speciation is considered to govern availability. In the water compartment, metal speciation can be tackled in a mechanistic way. A large number of computer programs are available to calculate the proportion of the metal species capable of entering the exposed organisms. The input to those calculations requires a quantification of a number of water chemical variables (pH, hardness, DOC, et cetera). For the soil and sediment compartments, the bioavailable fraction of the metals is, in general, empirically related to a number of soil and sediment characteristics (pH, cation exchange capacity, calcium content and such). Exposure of target species is further addressed by food-chain modelling, that is, a set of models that describes how toxicants taken up from the matrix are transferred by exposed biota to species on higher levels in the foodchain.

### 3.4.2 Statistics-based effect modelling and natural variability

Like in the exposure models, the effect-oriented models can be based on statistical patterns amongst the sensitivities of different organisms. "All animals are unequal" as far as the sensitivity to contaminants is concerned. Statistics-based effect-oriented models have been widely applied so far in the formulation of environmental policies.

Two model classes can be distinguished: statistical effect-extrapolation models and QSAR- (Quantitative Structure Activity Relationships) like models. Statistical extrapolation models are applied to estimate the concentration for which a certain percentage of the species in a

theoretical ecosystem is not exposed above their laboratory-determined no-effect concentration (HCx, the Hazardous Concentration for x percent of a species assemblage), or *vice versa* the percentage of species that likely is affected by a certain environmental concentration (PAF, the Potentially Affected Fraction). These models use the variability in sensitivity between species, which can be described by log symmetrical distributions (e.g. log normal, log logistic).

Posthuma et al. (2002b) have given a broad overview of options and limitations of this type of modelling and provided some examples of validation (Van den Brink et al. 2002a). An example of the dual use of the model for derivation of EQCs and for site-specific (retrospective) risk assessment is given in Figure 5.

QSAR-like models make use of large effect datasets to derive relationships between physico-chemical characteristics of a set of compounds and their (ecotoxicological) effects. These relations can be applied for the estimation of the effects of a new substance for which no substance-specific ecotoxicity data are available.

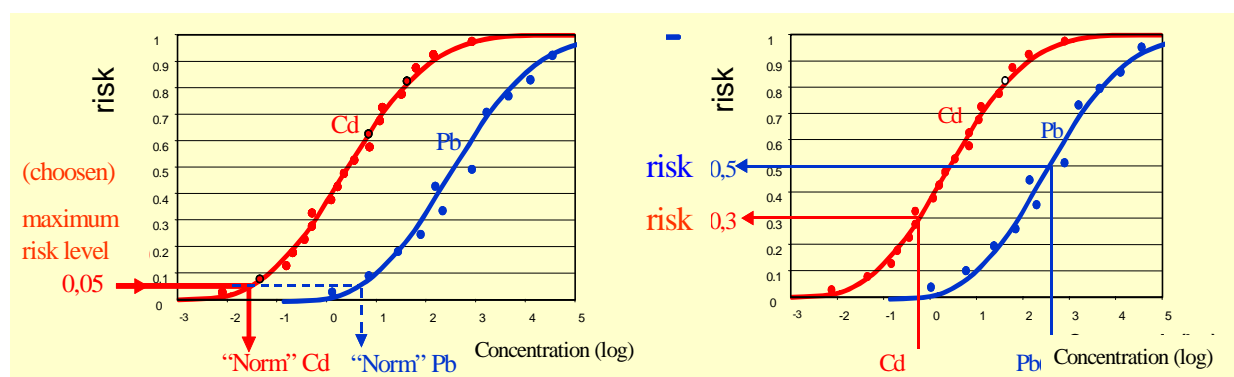


Figure 5. The dual use of Species Sensitivity Distributions as proposed by Straalen and Denneman (1989).

Left: derivation of EQCs for two compounds: by using the SSD of both compounds (Pb and Cd) and choosing a standard cut-off level of risks (5%), the generic EQCs of the two compounds are underpinned. Right: environmental contamination of a river with Cd and Pb can be recalculated into two measures of local risk (msPAF), that can be aggregated to an overall local risk level (following De Zwart and Posthuma 2005).

As a combination, the SSDs of a non-tested compound can be predicted by using patterns in the data set on tested compounds and tested species, as proposed by De Zwart (De Zwart 2002). In this case, the slope coefficient of the SSD was shown to be (grossly) related to the Toxic Mode of Action (TMoA) of the compound. When thus only the TMoA of a compound is known, it is feasible to predict the SSD characteristics of that untested compound and to predict (thus) provisional HCx and PAF values.

These statistical models are generic techniques that do not intend to estimate effects of substances on basis of mechanistic methodologies and consequently, they were not designed to be applied to problems that desire specific solutions. A statistical method, by its sole use in ecological risk assessment and associated environmental policies, does not change into an ecological method due to this. The method of SSDs has advantages in that it can be of help in



addressing environmental problems in many instances, but its clear disadvantage is that its output will always remain to be a statistical prediction.

### **3.4.3 Mechanism-based (ecological) models and biological phenomena**

Mechanistic models are generally based on species characteristics (population models) or on food chain or food web approaches to describe substance-fluxes and their effects through a predefined system that consists of relationships between species or ecological functions. From these models, effects of substances may be estimated for specific targets (i.e. certain species or functional groups), by which in turn more general assessment of risks can be derived when necessary.

From the point of view of providing a better understanding of the ecological phenomena that may occur, mechanistic methods may be preferred over statistical models. However, mechanistic models usually require a large amount of input data before they may be applied. Generally, these data are not available and exhaustive data-gathering projects are too time-consuming and expensive to fill in data gaps for many assessment problems.

Another aspect is that the validity of the results of mechanistic models is difficult to assess and the complexity of mechanistic models may be beyond our scientific knowledge, favouring the straightforward, simplistic statistical models for general ecotoxicological problems. To enhance the validity of mechanistic approaches, the results of assessment may be compared to observed effects in the field. However, these observed effects do not necessarily originate from toxicological stress which is only one of the many possible physical, chemical or biological causes of effects that may be detected. Consequently, it may be questioned if the mechanistic models may be validated at all, as long as data availability remains a source of concern.

### **3.4.4 Expert Models**

The last type of models is provided by the approach called “Expert models”. Expert models have been designed for decision-situations where decisions are made frequently, by different persons, for a commonly encountered problem. The approach is commonly used by physicians and judges, in order to identify human disease and to determine the punishment of e.g. speeding. In the case of an expert model, a database is used to “capture the past experiences” (e.g., the diagnosis of an illness by a physician and the verdicts of other judges), whereby others can use this database to diagnose or to decide on the new verdict. An expert model has been defined on the effects of pesticide in water bodies, e.g., those adjacent to sprayed fields (Van den Brink et al., 2002b). By using the expert system, PERPEST, risk assessors can predict the community-level impact of pesticide use, whether or not corrected by spray drift effects et cetera and to predict whether these effects remain lower than the acceptability limit. An example of a PERPEST-based prediction is given in Figure 6.

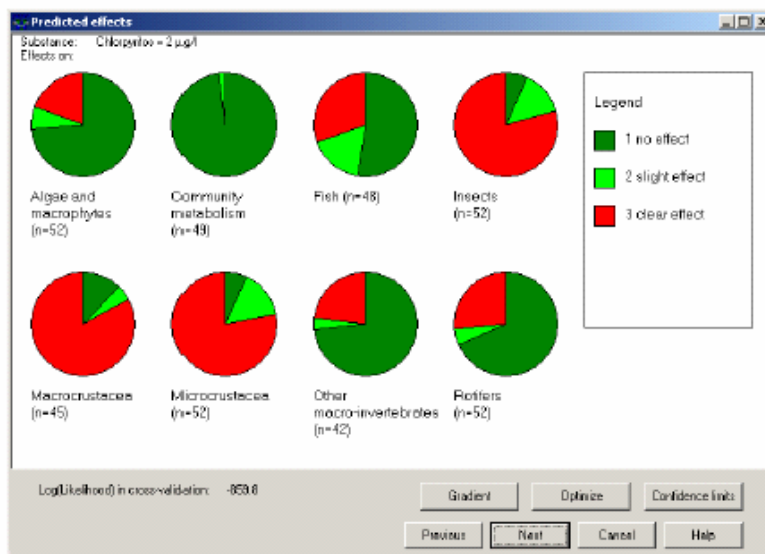


Figure 6. The prediction screen of PERPEST. After providing input data, the model predicts the impact on different species groups, in terms of magnitude of effects.

### 3.5 The choice of models and the toolbox concept

It seems to be impossible to determine in advance which type of models comes out best for a certain ecotoxicological problem and tiered approaches may be needed. To investigate whether the different types and sorts of models match the ecotoxicological data collected in several field studies *at all* is one of the reasons that the SSEO project has been initiated. From comparisons, it can be derived which models are *best* suited for certain types of policy problems and in how far *simple* models can be used despite the presence of better but more complex models. The main objective of this comparison is to generate an overview of the ecotoxicological models that may be applied to solve ecotoxicological problems and to arrange these models in order of suitability.

When made, such comparisons can be applied to develop the required decision-support toolbox for environmental management purposes, aiming at quantification of possible adverse effects posed by sites polluted with a mixture of contaminants, especially at low concentration levels. The validation project in which this is undertaken (in phase 2) aims at bringing together and integrating ecotoxicological models that are based on different concepts, integration level, systems and are developed for different problems (deterministic versus stochastic, general versus specific and terrestrial versus aquatic). In phase two of the SSEO-integration project, the tools from the toolbox will be parameterised and tested with the data that were gathered within the framework of the NWO Stimulation Program for System-oriented Ecotoxicological Research (SSEO).

### 3.6 Model criteria

The first selection criteria for choosing a model to be a tool in the toolbox is that sufficient information on the model has to be available from publications, reports or web sites (Pastorok et al., 2002). This enables to describe the model inputs and endpoints, the basic modelling approach, model equations and past uses of the model.

In this paragraph, a set of evaluation criteria is defined to give insight in the most important model characteristics of the models that are (provisionally) included in the toolbox (i.e., the limited toolbox considered in the SSEO framework). These criteria are described to enhance interpretation of the model descriptions. In subsequent paragraphs, each of the models is first introduced with a brief impression is given of the model's purpose and main applications, including the name of the developer of the model and the version number that was described. Model details are expanded in the accompanying tables on various aspects which may increase the comprehensibility of the models for potential users of the toolbox.

### 3.6.1 Scope

The scope refers to the purposes of the model for scientific and policy aims. In the table entry *Scope* the main applications of the model will be discussed and an overview is generated which defines the domain of the models regarding substances and ecosystems. Furthermore, it is noted to what extent the model is accepted for scientific and policy purposes.

### 3.6.2 Scale

The table entry *Scale* will present the time and spatial scales for which a model can be applied. It gives an overview whether the model is restricted to a certain time scale or location. The latter could refer to both a specific location for which the model was intended and to area sizes (e.g. spatial resolution). Furthermore, it is noted whether a model can be extrapolated to other time or spatial scales, which will improve its applicability and flexibility.

### 3.6.3 Realism

The *Realism* of the models is expressed in terms of how well a model represents reality. The first criterion that will be described is whether the model is based on empirical (i.e. statistical) or theoretical (mechanistic) basis. For both type of models, an overview is given of processes and mechanism that are ignored in the model which may have an influence on model outcomes or which hamper the use of the model for scientific or policy aims. Furthermore, the main assumptions are depicted so users can be facilitated to determine their faith in the model.

### 3.6.4 Input/Output

In the *Input/Output* section, the input parameters are presented which may serve as a handle for users to determine whether or not they have sufficient data to apply the model. Input parameters are split up in required parameters and optional parameters that may be entered to improve the reliability of and confidence in model outcomes. Furthermore, the benefits or improvements of model calculations are mentioned when these optional parameters are entered. The availability of input parameters is reported to state whether the model can be used for quick, initial assessments or only if preceded by extensive research to estimate parameter values. Moreover, if model calculations will only result in reliable results within certain ranges of the input parameters, these ranges will be reported. Some models leave the possibility to replace default parameter settings with user-defined parameter values. If so, these parameters are reported, including their default values. Besides input parameters, internal, intermediate model parameters that will be estimated may also be reported. Regarding output parameters, it is reported which parameters will be returned by the model and whether the model results appear in a graphical or numerical format.

### 3.6.5 Uncertainty

One of the major aspects of a model is how certain a user can be of the outcomes. Since models are simplifications of reality, it should be kept in mind that their results may not always agree with observations. This disagreement can be explained by uncertainty in the

estimation of input parameters or uncertainty about processes in the model itself. Various models take this uncertainty in input parameters or processes into account and propagate it throughout the model. The table entry *Uncertainty* discusses how uncertainty is included within each model and in the results of model calculation. Suggestions are given to reduce uncertainty in model estimates.

### **3.6.6 Calibration**

Most mechanistic models have been calibrated in the past to ensure optimum prediction precision and to get an idea of the scope and applicability of the model. This calibration could take place with data sets that are representative for the purpose of the model or by expert judgements. However, calibration is only useful if the calibration was performed within the same scope as the model is generally used. For instance, if calibration was performed with a certain substance or under specific environmental conditions, the model should not be extrapolated as such to other substances or environmental conditions, without investigating what the influence of this adaptation may be for model outcomes. Furthermore, if the model calibration was performed with an extensive dataset, whereas generally few data are available, the representativeness of the model calibration may also be mediocre. If the calibration process was reported in public literature, references are given for further information on the method of calibration.

### **3.6.7 Feasibility of model**

For potential users, the feasibility of a model may be the most important factor to select a specific model when several alternatives are available. The availability of a model is an important factor that determines the distribution and application of the model, which may help improving the implementation of underlying mechanisms in the model and its acceptance by third parties. The consistency and variability of model results are also important for the feasibility of the model. Large variations, high uncertainty of model outcomes and inconsistencies between model runs, will decrease the feasibility and faith in models. The latter may also be hampered by limited options to adapt a model to make it applicable for other purposes or environmental conditions. Model complexity and comprehensibility of underlying mechanisms may influence the usefulness of a model if users are not able to run the model without advanced programming or modelling knowledge. Good documentation of the model or setting up courses for novice users may aid potential users, although this may not be sufficient to catch up with more convenient models. The last aspect that may determine the convenience of using a model is the calculation efficiency, which refers to the preparation and calculation time after the required data has been collected.

### **3.6.8 Alternative models**

The models that were selected for the toolbox may not be the only models that may be applied for a specific ecotoxicological problem. To give potential users of the toolbox an overview of alternative ecotoxicological models that may be better suited for their problem or to discuss the differences between models that may be applied for a specific problem, alternative models are listed, together with the main differences with the model that may be included in the toolbox. If the model was compared with alternative models, the outcome of this comparison may also be presented. In addition, some models may be presented that can be used with the model of interest to generate input data or to perform further calculations with the outcome of the toolbox model. In some cases, other models preceded the model of interest and these previous models may be listed as well.

### **3.6.9 Development**

As stated in the introduction, most models are not finished as the process of development will continue endlessly. Therefore, insight is given in the options for improvements and future

plans and problems that might hamper developments. Furthermore, if a model is currently in an early development state, it may be possible to co-operate with users of the toolbox to improve the feasibility of the model or to develop new functionalities. Otherwise, users may awaiting these developments in their judgement of a model or anticipate on future features when planning their data collection.

### **3.6.10 References**

The last method to gain insight in the background of the selected models is to collect public literature about the model. In the table entry *Reference*, a list of the most important resources about these models is presented. These sources may consist of model descriptions, examples of model use and discussions on calibration and validation methods.



## 4. Model descriptions

### 4.1 General

This chapter gives an overview of the (effect) models, as the basic composition of a toolbox design. Only those models that are well documented in the open literature and have proven their applicability and usefulness for certain assessment problems will be considered. As the RIVM/RIZA/Alterra consortium responsible for the development of the toolbox is more aware of their in-house models, the selection of models may be somewhat biased towards the models that have been developed by these institutes. The emphasis is mainly towards effects. The models that were selected are: (1) ETX2.0 (2) OMEGA123, (3) IQ-TOX, (4) HERBEST, (5) OMEGA45, (6) PODYRAS, (7) CATS and (8) PERPEST.

The model descriptions provided below are based on the criteria that were introduced in the previous chapter. Readers should keep in mind that these descriptions gives a state-of-the-art of these models at the moment that these evaluations were performed. Future developments or modifications to the model may lead to different evaluation statements. Furthermore, one should keep in mind that each model is described by its developer, so users should always carefully evaluate the information on models and judge whether or not the model is applicable to a specific ecotoxicological problem.

### 4.2 Statistics-based effect models

#### 4.2.1 ETX-2.0

*ETX 2.0* is a general assessment model, offering the opportunity to apply statistical theory common to species sensitivity distributions (SSD, see Posthuma et al. (2002b) and Figure 5). The model can serve for two purposes:

1. The derivation of Hazardous Concentrations (HCx), of which the HC5 and HC50 are commonly used as risk limits underpinning the derivation of EQCs
2. Quantitative Risk Assessment (QRA), whereby an existing contamination level in the environmental is expressed in quantitative risk terms (PAF, the locally Potentially Affected Fraction of species)

Any ecotoxicity input data can be applied in the lognormal model that is used to describe the variation in sensitivities among tested species. *ETX 2.0* can be used to calculate the following items (by A. Wintersen, T.P. Traas and L.Posthuma, on Version 2.0):

- The program calculates a normal distribution through the data set.
- The program shows the results of three goodness-of-fit tests that can be used to decide whether your data follow a normal distribution. The three tests are known as Kolmogorov-Smirnov anderson-Darling and Cramér-von Mises.
- The program calculates the median HC5 (hazardous concentration for 5 percent of the species, i.e., the 95% protection level) plus its two-sided 90% confidence limit and the median HC50 (basis for the Dutch Intervention Value) plus its two-sided 90% confidence limit. At the HC5 and HC50, the corresponding median FA (fraction affected) is given (i.e. 5% and 50%, respectively) together with its two-sided 90% confidence limit.

- The program also calculates the Potentially Affected Fraction of species at a given degree of environmental exposure (not necessarily being the HC5 or HC50), through which one can perform so-called quantitative risk assessment
- Results are graphically presented in a histogram and in a cumulative density function (the latter is commonly referred to as SSD).

<b>Scope</b>	
Use in policy making	The model is used in the setting of Dutch Environmental Risk Limits
Model	SSD: log-normal
Substances	Any substance for which 3 or more ecotoxicity data are known
Ecological	
Acceptance	The use of SSD's is widely accepted in Dutch policy making.
Predictive/Comparative	Predictive

<b>Scale</b>	
Time	
Space	

<b>Realism</b>	
Empirical/Theoretical basis (i.e. is the model based on a statistical or on a mechanistic approach?)	The model is based on statistical assumptions.
Missing processes	
Assumptions (and their consequences)	.- Species sensitivities are log-normally distributed - Laboratory toxicity tests are representative of field toxicity

<b>Input/Output</b>	
Input variables (units)	Ecotoxicity endpoint data (NOEC, EC50,...)
Minimum requirements	3 data points
Optional	A single Predicted Environmental Concentration (PEC), or a collection of exposure data may be entered in order to determine the Fraction Affected. Data can be labelled optionally in order to visualize subgroups (e.g. taxonomic groups) within the data
Benefit of collecting more data / Data efficiency	The confidence limits of the fraction affected will be reduced
Data availability	Good for aquatic species, reasonable for terrestrial species and processes.
Range of parameter values that may be entered to obtain reliable results	3 – 200 toxicity data values. 1 – 200 exposure data values.
Internal parameters (units)	Any
Which parameters are estimated within the model that could have been obtained by other means (i.e. empirical data)?	Optionally the spread of the distribution can be estimated by the model (small sample approach).
Output variables (output)	Hazardous concentrations (HC5, HC50), Fraction Affected, Goodness-of-fit tests, SSD, Joint Probability Plot
Graphics/Numerical output	

<b>Uncertainty</b>	
Model outcomes	The uncertainty is estimated based on the sample size.
Is reduction of uncertainty achievable?	Reduction of uncertainty is possible by entering more data.



<b>Validation</b>	
Status	The concept of SSD's has been validated within numerous projects. Validation is still ongoing. Conceptual tiered models exist of which validation is an integral part (TRIAD).
Scope of validation (representativeness validation study)	
Documentation of validation	
<b>Feasibility of model</b>	
Reproducibility of results (Consistency & Variability)	
Flexibility	
Complexity/Comprehensibility	The model is not complex and uses well known ecotoxicological principles.
Model availability	The model is freely available for non-commercial purposes.
Calculation time	Milliseconds
<b>Alternative models</b>	
Alternatives	Other models (e.g. Omega123) incorporate the SSD methodology.
Links/Co-operation with other models:	
Reputation in comparison with alternatives:	Good
<b>Development</b>	
Options for improvement(s):	Mixture toxicity, other types of distributions
Future plans:	
<b>Documentation</b>	
Van Vlaardingen et al. (2004)	

#### 4.2.2 OMEGA123

The RIZA model *Optimal Modelling for Ecotoxicological Applications*, OMEGA, is a relatively simple model, developed to answer scientific questions put forward by water pollution management.

The benefits of the use of OMEGA can be described in terms of the (combination of) advantages that OMEGA has in comparison with most other ecotoxicological models (by M. Beek, RIZA and A.J. Hendriks, Radboud, 2000, version OMEGA123, 4.0):

- OMEGA covers the whole cause-effect chain from accumulation kinetics to population dynamics
- OMEGA uses classical mechanism-based equations that have been calibrated on/validated with thousands of data
- OMEGA allows application to poorly investigated substances and species because parameters have been linked to well-known characteristics such as octanol-water partition ratio  $K_{ow}$ , species trophic position and weight
- OMEGA is well documented in open literature.
- Apart from a general scientific aim “to keep models as simple as possible”, application of relatively simple models may help to reduce uncertainty too (Håkanson, 1995).
- The OMEGA model is/will be linked to environmental fate models for floodplains in national rivers (BIOCHEM) and for regional water bodies (BOREAS)

After an input of concentrations in water, sediment or soil by the user, the model:

- calculates the ratios of the concentration versus the quality standard;
- calculates the fraction endangered species (PAF);
- gives the problem substances and vulnerable species with high PAF.

An example of output for one compound is provided in Figure 7.

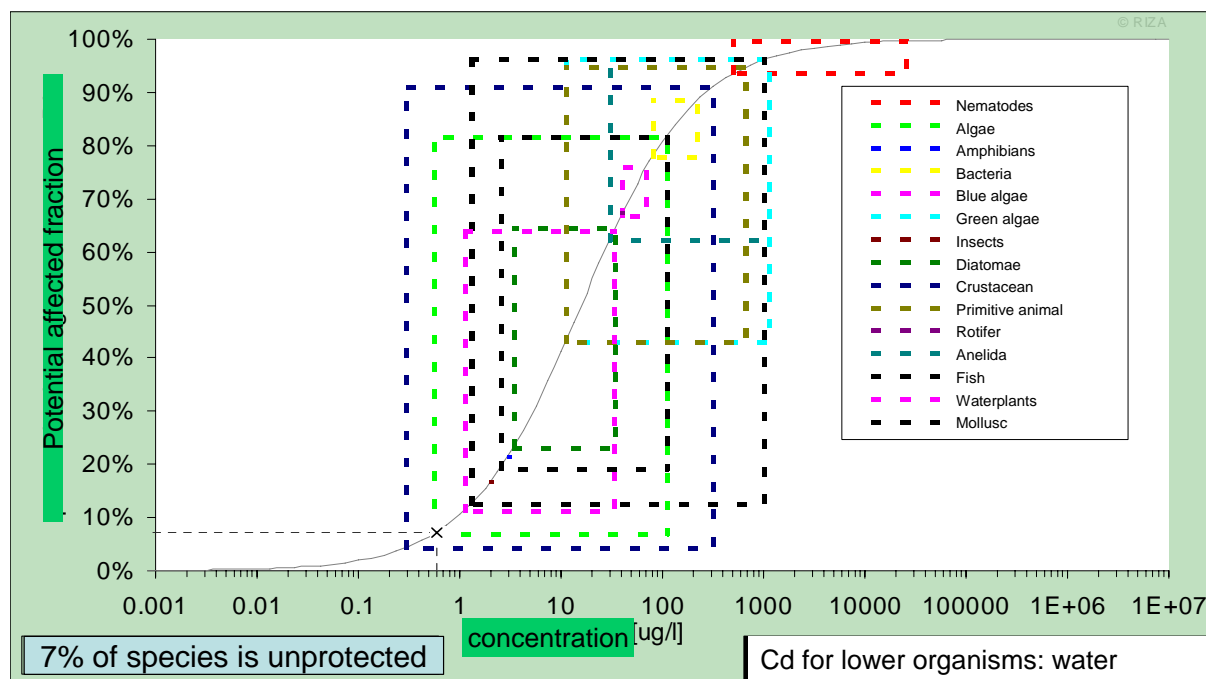


Figure 7. Example of output from OMEGA123 for Cd for lower organisms in water. The SSD is constructed from an array of species types, for which the outer ranges of sensitivity variation are shown by the boxes. At a concentration of approx. 0.7 microgram per liter, the proportion species exposed beyond their NOEC is expected to be 7%, concerning likely NOEC-exceedance for two groups of species specifically.

Scope	
Use in policy making	OMEGA123 may be used for national, regional and local risk assessments.
Model	The model will return a preliminary indication of substances and species that need to be investigated in detailed empirical or theoretical studies.
Substances	The model may be applied to all substances with sufficient toxicity data that were gathered within the scope of the project 'Setting Integrated Environmental Quality Standards'.
Ecological	The model can be applied to several ecosystem types.
Acceptance	It is widely recognised (for both scientific and policy purposes) as an initial estimator of ecological risk.
Predictive/Comparative	Both.

Scale	
Time	The aspect of time-dependent exposure levels or effects are ignored in OMEGA123.
Space	The use of local concentrations as input parameters allows for site-specific risk estimations.

Realism	
Empirical/Theoretical basis (i.e. is the model based on a statistical or on a mechanistic approach?)	OMEGA123 is a statistical extrapolation model.

Missing processes	OMEGA123 is a generic tool that lacks mechanisms for detailed analyses, such as bio-availability.
Assumptions (and their consequences)	An overview of assumptions and their consequences is given in Posthuma et al. (2002).

### Input/Output

Input variables (units)	
Minimum requirements	Environmental concentrations and the compartment in which the substance is present.
Optional	None.
Benefit of collecting more data / Data efficiency	The model uses a fixed set of ecotoxicological data that cannot be modified by users. Data collection by the developer results in more correct assessments.
Data availability	Generally, there are no problems with data availability.
Range of parameter values that may be entered to obtain reliable results	No input of parameter values (concentrations only)
Internal parameters (units)	None.
Which parameters are estimated within the model that could have been obtained by other means (i.e. empirical data)?	None.
Output variables (output)	The potentially affected fraction (PAF) of species, problem substances and high-risk, vulnerable species and taxonomic groups.
Graphics/Numerical output	Numerical PAF-values and graphical presentation of SSD-curves and vulnerable groups.

### Uncertainty

Model outcomes	Uncertainty in model estimations is ignored.
Is reduction of uncertainty achievable?	Gathering more toxicity data can reduce uncertainty.

### Validation

Status	Although the model itself has not been validated at this moment, rudimental validation studies have been performed for SSD concepts.
Scope of validation (representativeness validation study)	Not applicable.
Documentation of validation	Not applicable.

### Feasibility of model

Reproducibility of results (Consistency & Variability)	Model outcomes are completely reproducible.
Flexibility	The model can easily be adapted to different environmental conditions.
Complexity/Comprehensibility	OMEGA123 is a relatively simple model, which can be understood by anyone with basic knowledge of statistics.
Model availability	Yes, the model can be obtained free of charge from RIZA, contact person M. Beek
Calculation time	Model calculations are completed within seconds.

### Alternative models

Alternatives	Yes, see Posthuma et al. 2002.
Links/Co-operation with other models:	OMEGA123 may be used with chemical and ecological models.
Reputation in comparison with alternatives:	Not applicable.

### Development

Options for improvement(s):	Several options for improvement exist, including validation, collection of more data and refinement of combination toxicity.
Future plans:	Regular use and low-profile development.

### Documentation

Beek et al. (2002); Beek and Hendriks (2001); Durand (2001, (In Dutch)); Durand (2000); Knoben et al. (1998); Beek and Duivenvoorde (1998); Beek and Knoben (1997)	
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### 4.2.3 IQ-TOX

The RIVM model *IQ-tox* (*Instrument for the Quantification of Toxic Stress*) is, at present, a modelling philosophy rather than an operational model ready for use by third parties. It concerns the same modelling ‘engine’ as ETX2.0 and OMEGA123, viz. Species Sensitivity Distributions (SSD, see Posthuma et al., 2002b).

The idea of an SSD is simple: an SSD represents the spread of sensitivities amongst different organisms as measured in laboratory toxicity tests. These shows that ‘all animals [organisms] are unequal’: each species shows a particular (in)sensitivity. For example: insects are more sensitive for insecticides than plants, plants show higher effects when exposed to photosynthesis inhibitors. When the distribution of sensitivities is plotted, one can derive either *Generic Environmental Quality Criteria* or *Site-specific estimates of (mixture) risks*. Thereby, establishing a strong conceptual link between setting quality standards and assessing local risk.

The statistical meaning of PAF and msPAF is the following. Say, the msPAF for a soil is calculated as 25% based on SSDs that are constructed from the 100 available NOEC-values of each of the compounds in the mixture. That is: if one would rear all 100 species in the contaminated soil, one would predict that for 25% of *those* species the NOEC would be exceeded. Similarly, when the SSD would have been constructed from LC50s, one would predict substantial mortality (>50% of the individuals would die) in 25% of the species and less or no mortality in other species. Whether the test species are representing the species in natural ecosystems is under debate. However, it is clear that high (ms)PAF values identify sites where subselections of the tested species would not flourish and (thus) that the method itself might have limitations in terms of ecological realism, the output can be used for ranking of (most affected) sites, of (most toxic) compound and of (most affected) species groups.

Site-specific assessment of the environmental risks of local contaminant mixtures in water, sediment or soil is the target of *IQtox modelling*. There is a large number of contaminated sites, water bodies and sediments in the Netherlands. RIVM-strategic research is focused on the development of methods to quantify local risks at those sites. *IQtox* addresses local exposure concentrations (by applying environmental chemical analyses of exposure), local risk per compound (by SSDs), local risk of mixtures (by applying mixture extrapolation rules) and eventually thus the local ecological risk of a mixture for a certain ecosystem.

The *IQtox* concept has many issues in common with *ETX2.0* and *OMEGA123* modelling. However, it differs from *ETX2.0* and *OMEGA123* in the following ways:

- input data: unlike OMEGA123, it has no predefined set of ecotoxicity data from which risks are calculated; these data originate from (preferably) the RIVM e-toxBase (a toxicity database with > 166.000 data on different compounds, species and exposure levels, see Wintersen et al. (2004)), which means that not only NOECs can be used, but also EC50s, LC50s, et cetera
- Amongst other, it applies *ETX2.0* as modelling tool, i.e., it applies a lognormal SSD model when *ETX2.0* is used, but it does not necessarily use that specific model for the SSD; it can use other SSD-mathematical models when those apply better to the data
- Attention is paid to local exposure-modifying conditions, whereby it currently applied expert judgement and tiered protocols according to De Zwart et al (2004)
- calculates the fraction endangered species (PAF) per compound

- calculates the fraction of endangered species (msPAF) for whole mixtures, according to methods proposed by (Traas et al. 2002a), Posthuma (Posthuma et al. 2002a), Zwart (De Zwart and Posthuma 2006 accepted)
- can take account of the specific Toxic Mode of Action of compounds (e.g. insecticides, photosynthesis inhibitors, et cetera)
- gives the problem substances and vulnerable species

The *IQtox* idea has not yet fully matured into a standardized toolbox item, since it is focused on giving tailored answers to specific problems. *IQtox*-based assessments are currently done by experts, e.g. to construct national trends analyses (e.g. for pesticide use in The Netherlands to construct spatial maps of toxic pressure (e.g. (De Zwart 2003)), for LCA (Huijbregts et al. 2002) and for various toxic-compound trend indicators. Various validation studies have shown that msPAF-values can be used for *relative* risk ranking, e.g., to identify the sites of a large set that are likely most affected by the contaminant mixture. A recent paper concerning validation analyses of the *IQTox* approach has been made, using field monitoring data – which implies analyses of toxicant effects in multiple-stress conditions (Posthuma and De Zwart, in press), see also Appendix 1.

Absolute risk ranking might be beyond the intrinsic characteristics of the method: since the method is *based* on statistics and ecotoxicity in the laboratory, there are intrinsic limitations as to its absolute ecological relevance. Although not a toolbox to be used for third parties in regular assessments, the *IQtox* approach is implemented in the assessment of toxic risks of spreading (slightly) contaminated sediments on land (Posthuma et al. 2005), under the special acronym *IRAsed.v1*. In that Integrated Risk Assessment model (based on *IQtox*), not only ecosystems risks were evaluated, but also risks to agricultural products and to exposed humans (see Figure 8).

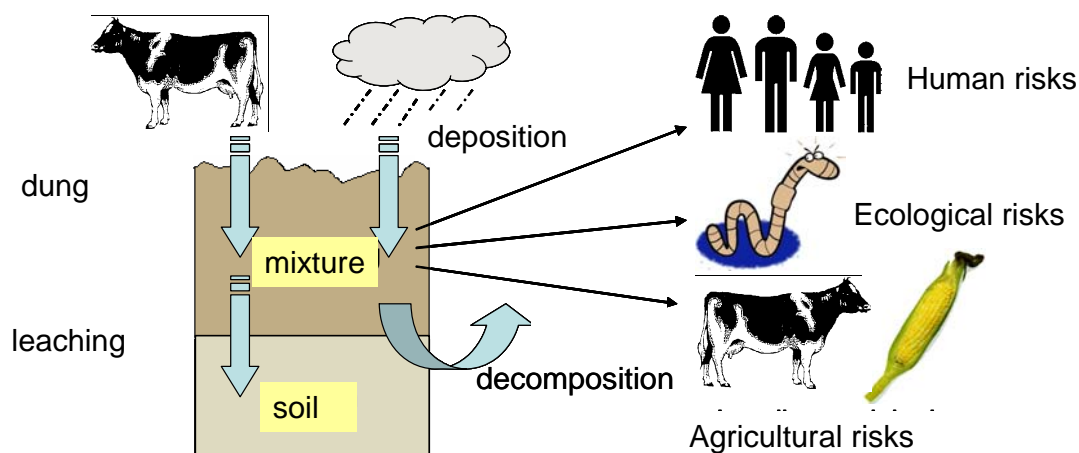


Figure 8. The site-specific approach of *IRAsed*, a model developed to assess the site-specific risks of deposition of sediment on land. Ecological risks were quantified with SSDs according to De Zwart and Posthuma (2005) and Figure 5.

<b>Scope</b>	
Use in policy making	IQtox may be used for national, regional and local risk assessments, for deriving Environmental Quality Objectives and for site-specific assessments
Model	The model will return a preliminary indication of the most affected sites, most potent substances and most affected species groups that might be further investigated in detailed empirical or theoretical studies
Substances	The model may be applied to all substances with sufficient toxicity data (as present in the RIVM e-toxBASE), or even to compounds where such data lack. In such cases, one can use surrogate data, as a consequence of the fact that SSDs are 'predictable' within e.g. a group of compounds (like in QSAR)
Ecological	The model can be applied to several ecosystem types
Acceptance	It is widely used (for both scientific and policy purposes) as an initial estimator of ecological risk and is applied in monitoring networks (to analyse temporal and spatial trends), in LCA, to support legal procedures
Predictive/Comparative	Both

<b>Scale</b>	
Time	The aspect of time can be addressed by choosing the most relevant data from the RIVM e-toxBASE, that is: similar exposure period in laboratory toxicity tests as in the problem to be assessed
Space	The use of local concentrations as input parameters allows for site-specific risk estimations and those local concentrations are preferably modified so as to estimate the available fraction.

<b>Realism</b>	
Empirical/Theoretical basis (i.e. is the model based on a statistical or on a mechanistic approach?)	IQtox is a statistical extrapolation model, although it is made to encompass concepts and data from environmental chemistry (exposure assessment), toxicology (modes of action) and ecology (particular sensitivity of species, e.g., insects for insecticides).
Missing processes	Ecological interactions are not covered; the final response in the field is either reinforced by ecological interactions (in the high exposure range: a cascade of secondary responses might follow, e.g. when prey species are most sensitive), or counteracted by interactions (e.g., ecosystem resiliency)
Assumptions (and their consequences)	An overview of assumptions and their consequences is given in Posthuma et al. (2002).

<b>Input/output</b>	
Environmental concentrations and the compartment in which the substance is present, combined with data that modulate true exposure (sorption to the medium due to e.g. pH, organic matter content).	
Minimum requirements	None.
Optional	Various Tiers can be developed, depending on the specificity of the problem formulation, e.g.: account yes/no for specific Toxic Modes of Action; account yes/no for exposure effects induced by the medium.
Benefit of collecting more data / Data efficiency	Generally, there are no problems with data availability.
Data availability	Measured total concentrations are mostly available; for many problematic compounds, sufficient ecotoxicity data are available (much more than the sub-selection chosen to use in the INS-project).

Range of parameter values that may be entered to obtain reliable results	None.
Internal parameters (units)	None.
Which parameters are estimated within the model that could have been obtained by other means (i.e. empirical data)?	The potentially affected fraction (PAF or msPAF) of species, problem substances and high-risk, vulnerable species and taxonomic groups.
Output variables (output)	Numerical PAF-values and graphical presentation of SSD-curves and vulnerable groups.
Graphics/Numerical output	

### Uncertainty

Model outcomes	Uncertainty can be shown, e.g. when using the standard modelling tool ETX (2.0)
Is reduction of uncertainty achievable?	Yes, by looking at specific Toxic Modes of Action and the associated misfit in the SSDs (fit evaluation protocols are available in ETX 2.0), by selecting data that are more appropriate to the assessment problem (e.g. EC50s instead of NEOCs when exposure levels are high)

### Validation

Status	SSD-validation studies have shown that effects in field ecosystems and/or mesocosm usually start at (much) higher concentrations than the HC5. Further, SSD-validation studies have looked into the association between prediction and observed effects in field gradients. There seems a positive association between msPAF and biodiversity effects, but (in addition) there is much statistical 'noise' due to other stress factors.
Scope of validation (representativeness validation study)	Water and soil studies and a study on indirect effects (that is: butterflies responding to plant species that respond to metal exposure).
Documentation of validation	Various open literature publications

### Feasibility

Reproducibility of results (Consistency & Variability)	Model outcomes are completely reproducible when the same exposure models, SSDs and input data are used; method can be standardized for frequently encountered assessment problems (e.g., LCA protocol).
Flexibility	The model can easily be adapted to different environmental conditions.
Complexity/Comprehensibility	IQtox is a relatively simple model, which can be understood by anyone with basic knowledge of statistics and with insight in the processes of exposure and intoxication.
Model availability	The model can be applied by RIVM experts, but standardized formats for use by third parties are being developed, e.g. for sediment quality assessment to decide whether sediments can be deposited on land
Calculation time	Model calculations are completed within seconds.

### Alternative models

Alternatives	Yes, see (Posthuma et al., 2002b; Traas et al., 2002b).
Links/Co-operation with other models:	IQtox may be used with chemical and ecological models
Reputation in comparison with alternatives:	Not determined

### Development

Options for improvement(s):	Several options for improvement exist, including further validation, collection of more input data and refinement of exposure assessment and mixture toxicity
Future plans:	Under development in the Spearhead for RIVM. Strategic Research 2003-2006

<b>Documentation</b>	
Model and model use: Traas et al. (2002b); Posthuma et al. (2002a);(Posthuma et al. 2002b); De Zwart (2002); Aldenberg and Luttik (2002); Huijbregts et al. (2002); Posthuma et al. (2003a); (Posthuma et al. 2003b); Posthuma et al. , Posthuma et al. (2003b); De Zwart et al. (2005 accepted); De Zwart (2004); De Zwart and Posthuma (2004); Posthuma and De Zwart (2005); (Mulder et al. 2004)	
Database for input toxicity data: Wintersen et al. (2004)	

## 4.3 Mechanism-based models

### 4.3.1 HERBEST

The HERBEST (In Dutch: “HERstelmodel BESTrijdingsmiddelen”, or Recovery Model for Pesticides) model is a simple model describing the acute effects and recovery of chemical-stressed keystone populations in aquatic ecosystems. It can be used to get a first impression, how long an impact of a chemical application will last and/or can fill in gaps in collected (semi-)field data. The aim of the model is to predict direct effects and recovery of a population using a minimum of input data. The input of the model is pesticide concentration (measured or predicted by a fate model), a species name, the toxicity of the particular chemical for that species (EC50 and NOEC) and some life cycle characteristics of the species (the number of emergence-periods per year, the ability to migrate and the reproduction rate). The output consists of the response of the species in time and its recovery time. The model is integrated in a user friendly user interface. The evaluation of mixtures of chemicals can easily be incorporated in the program (by P. van den Brink).

<b>Scope</b>	
Use in policy making	HERBEST can be applied for the population-level risk assessment of pesticides, e.g. for their registration
Model	Freely available with Graphical User Interface
Substances	Pesticides
Ecological	Yes includes life cycle characteristics
Acceptance	Yes, it is scientifically accepted to use life cycle characteristics to predict response of species to pesticide stress
Predictive/Comparative	Both

<b>Scale</b>	
Time	weeks to year
Space	Ditch

<b>Realism</b>	
Empirical/Theoretical basis (i.e. is the model based on a statistical or on a mechanistic approach?)	Theoretical
Missing processes	Stochasticity, only most important life cycle characteristics are yet incorporated, no chronic toxicity, external recovery
Assumptions (and their consequences)	No chronic toxicity, all life stages are equally sensitive

<b>Input/output</b>	
Input variables (units)	



Minimum requirements	Nominal concentration, DT50, sensitivity and life cycle characteristics of species
Optional	Concentration dynamics
Benefit of collecting more data / Data efficiency	Data needed for insight in life cycle characteristics and validation
Data availability	Good for fate of chemicals and sensitivity. More difficult for life cycle characteristics
Range of parameter values that may be entered to obtain reliable results	Depends on parameter
Internal parameters (units)	Initial concentration ( $\mu\text{g/L}$ ) DT50 (days) Population growth rate (1/day) Recolonisation period (date) Duration of recolonisation event (days) Date for $t=0$ (date) Recovery threshold (%) EC50 ( $\mu\text{g/L}$ ) Slope at EC50 (-) NOEC ( $\mu\text{g/L}$ )
Which parameters are estimated within the model that could have been obtained by other means (i.e. empirical data)?	Recovery moment can also be assessed in outdoor mesocosm experiments
Output variables (output)	Recovery moment (days)
Graphics/Numerical output	Both

**Uncertainty**

Model outcomes	Uncertainty not yet incorporated
Is reduction of uncertainty achievable?	Yes, uncertainty in input parameters can be included

**Validation**

Status	Partly, model ideas based on results of mesocosm experiments
Scope of validation (representativeness validation study)	Many mesocosm experiments
Documentation of validation	Not yet

**Feasibility of model**

Reproducibility of results (Consistency & Variability)	Consistent
Flexibility	Not so flexible
Complexity/Comprehensibility	Simple model
Model availability	Freely available via <a href="http://www.herbest.alterra.nl">www.herbest.alterra.nl</a>
Calculation time	Seconds

**Alternatives**

Alternatives	None
Links/Co-operation with other models:	Can be linked to fate model TOXSWA
Reputation in comparison with alternatives:	Unknown because of lack of known alternatives

**Developments**

Options for improvement(s):	External recovery, more life cycle characteristics, probabilistic input
Future plans:	Validation using mesocosm data, external recovery, more life cycle characteristics

**Documentation**

Van den Brink and Kuyper (2001). The Users Manual of the program is incorporated in the graphical user interface
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### 4.3.2 OMEGA45

OMEGA45 is a model that covers the whole cause-effect chain from accumulation kinetics to population dynamics. It uses classical mechanism-based equations that have been calibrated on and validated with thousands of data. OMEGA45 allows application to poorly investigated substances and species because parameters have been linked to well-known characteristics of chemicals (e.g. octanol-water partition coefficients) and species (e.g. trophic position and weight).

Generally, it will be applied to calculate the accumulation kinetics and population development of substances and species selected to be of concern in generic assessments. These species and substances may be identified with OMEGA123. Past development and application were focussed on the kinetics of stable and labile substances in aquatic, benthic and terrestrial food chains and the dynamics of monotrophic systems. Present development and application are focussed on (by A.J. Hendriks, RIZA / Radboud University Nijmegen):

- kinetics of non-traditional substances: toxins, oestrogens, pharmaceuticals;
- toxicokinetics of internal body burdens;
- dynamics of ditrophic systems (e.g. oscillation periods of phyto-zooplankton).

<b>Scope</b>	
Use in policy making	OMEGA45 may be applied for: <ul style="list-style-type: none"> <li>- the protection of species;</li> <li>- nature development;</li> <li>- the identification of problematic substances;</li> <li>- the prediction of population development of endangered species that may be rehabilitated;</li> <li>- the identification of sources of disturbances in populations or communities;</li> <li>- the comparison of toxicant and non-toxicant stress.</li> </ul>
Model	It may be used to integrate various data, identify outliers, select species and substances which require additional (empirical) research and to combine toxicant and other stressors.
Substances	OMEGA45 may be applied to: <ul style="list-style-type: none"> <li>- stable substances like as PCBs and metals;</li> <li>- labile substances like some pesticides;</li> <li>- non-traditional substances like toxins, oestrogens, pharmaceuticals, etc.</li> </ul>
Ecological	Development for aquatic, marine and terrestrial communities. Validation, however, is limited to rivers, lakes, estuaries and their floodplains.
Acceptance	Scientifically: equations are widely applied around the world and model parameters have extensively been calibrated in scientific publications. Policy-making: not applicable.
Predictive/Comparative	OMEGA45 is a predictive model.

<b>Scale</b>	
Time	The time scale of the model ranges from minutes to ages, depending on the processes simulated.
Space	It is applicable to any system, although validation is limited to rivers, lakes and their floodplains.
Restrictions or possibilities for extrapolation to other scale(s) (time, space)	No restrictions in time or space.

<b>Realism</b>	
Empirical/Theoretical basis (i.e. is the model based on a statistical or on a mechanistic approach?)	OMEGA45 is a mechanistic model, which input parameters are obtained by statistical analysis.
Missing processes	Several processes are ignored, such as: <ul style="list-style-type: none"> <li>- biotransformation is not predicted but has to be invoked;</li> <li>- interaction with other communities.</li> </ul>
Assumptions (and their consequences)	Several assumptions form the foundation of this model. These assumptions have described in detail in various papers (see below).

<b>Input/output</b>	
Input variables (units)	
Minimum requirements	Substance and species names, concentration in one abiotic compartment.
Optional	see data availability
Benefit of collecting more data / Data efficiency	Collecting more data should reduce variability and improve the predictive power of the model.
Data availability	The model provides default values for all parameters, to be modified by user if reliable information is available. All parameters values are directly or indirectly (after calibration) obtained from data.
Range of parameter values that may be entered to obtain reliable results	The model provides default values for all parameters, to be modified by user if reliable information is available.
Internal parameters (units)	The model provides default values for all parameters, to be modified by user if reliable information is available.
Which parameters are estimated within the model that could have been obtained by other means (i.e. empirical data)?	The model provides default values for all parameters, to be modified by user if reliable information is available. All parameters values are directly or indirectly (after calibration) obtained from data.
Output variables (output)	The model results are environmental concentrations (ug/kg) and population density (# or kg/km <sup>2</sup> or as fraction of control).
Graphics/Numerical output	The model returns both numerical and graphical output data.

<b>Uncertainty</b>	
Model outcomes	Uncertainty is not yet quantified.
Is reduction of uncertainty achievable?	Yes, by refinement of equations and additional calibration.

<b>Validation</b>	
Status	Accumulation validated for many aquatic and terrestrial species in or along rivers and lakes. Population development, however, has been validated for a few species only. The model was calibrated using empirical data.
Scope of validation (representativeness validation study)	The model has been validated for traditional toxicants and species. The model calibration was comparable to normal model use.
Documentation of validation	Well-documented (see below).

<b>Feasibility of model</b>	
Reproducibility of results (Consistency & Variability)	OMEGA45 is a deterministic model.
Flexibility	The model may easily be adjusted to specific aims and circumstances.
Complexity/Comprehensibility	Complete model has to be run by experts, but individual equations can be used by scientists from publications.
Model availability	The model is available for third parties but currently lacks a good documentation. So far, third parties use specific parts of the model for specific purposes (e.g. food chain accumulation, otter population development) by implementing formulas and parameters in their own programs.
Calculation time	Short.

<b>Alternative models</b>	
Alternatives	Formulas are traditional, some have been implemented by others as well. OMEGA45 is unique in the sense that default values are provided for parameters by linking them to well-known properties such as species weight or octagonal-water partition coefficients.
Links/Co-operation with other models:	OMEGA45 may be used in combination with chemical and ecological models, such as environmental fate models for floodplains in national rivers (BIOCHEM) and for regional water bodies (BOREAS)
Reputation in comparison with alternatives:	The model has been compared to models for specific foodchains. In general, deviations between the models were than deviations between model predictions and empirical data.

<b>Developments</b>	
Options for improvement(s):	The model may be enhanced by including dynamics of multitrophic systems.
Future plans:	Future development and application are focussed on dynamics of multitrophic systems (e.g. diversity).

<b>Documentation</b>	
Hendriks and Heikens (2001); Hendriks et al. (2001); Heikens et al. (2001); van der Linde et al. (2001); Smit et al. (2001); De Jonge et al. (2000); Heikens (1999); Hendriks (1999); Hendriks (1998); Hendriks et al. (1998); Hendriks and Van de Guchte (1997); Hendriks (1996); Hendriks and Enserink (1996); Gerrits and Hendriks (1995); Hendriks (1995a); Hendriks (1995b); Hendriks (1995c); Hendriks (1995d)	

### 4.3.3 PODYRAS

*PODYRAS* (Population Dynamical Risk Assessment model Series) has been developed to assess the impact of chronic pollutants on species in a terrestrial food-chain with the emphasis on priority species such as protected and red-list species. An earthworm model forms the first node in the food-chain, with this model bio-accumulation and the population level effects of pollutants on earthworms can be assessed. The second node in the food-chain is optional depending on the predator species in question. Models have been developed for the protected species badger and godwit and for the common shrew. *PODYRAS* is a deterministic analytic model (implying the mathematical tractability of its results) which is strongly based on the ecology of the analyzed species (by C. Klok, Alterra, 2000). An example of *PODYRAS*-principles and output is provided in Figure 9.

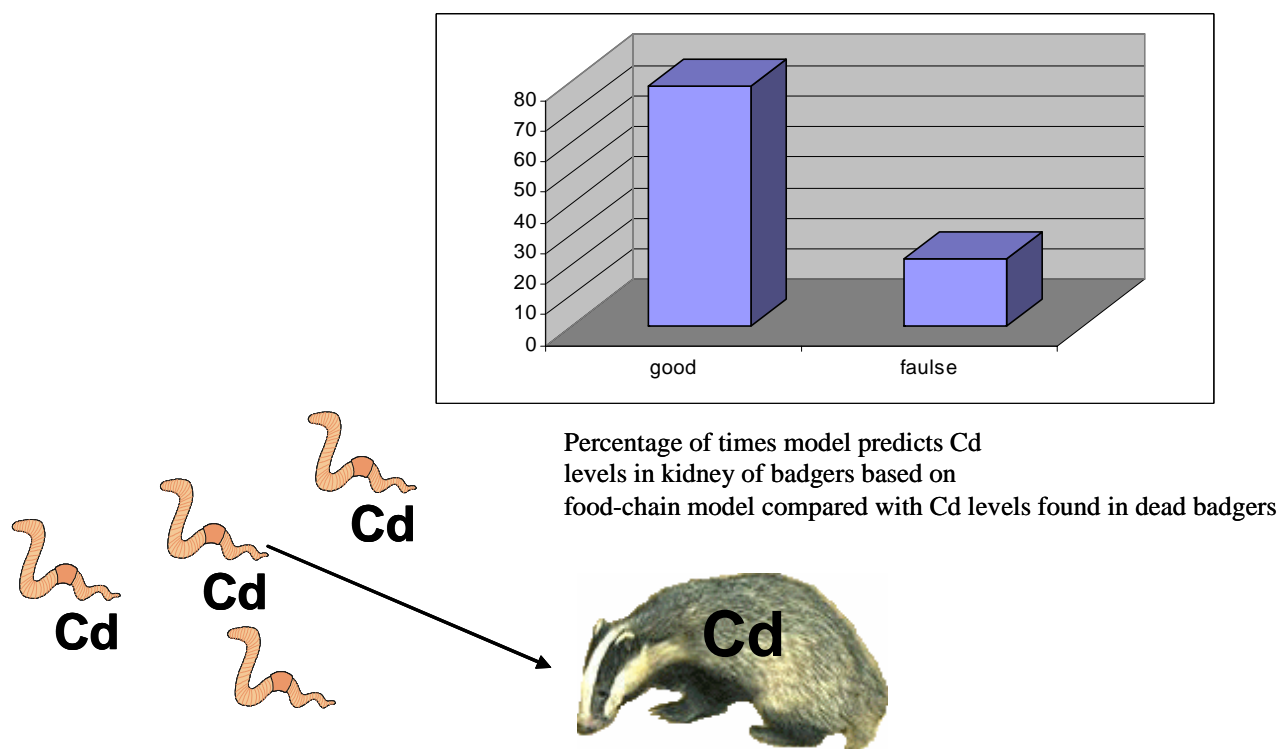


Figure 9. Principles and example-output of PODYRAS.

<b>Scope</b>	
Use in policy making	PODYRAS may be applied for <ul style="list-style-type: none"> <li>a- diagnosis of polluted sites;</li> <li>b- forecast in nature development</li> <li>- bioaccumulation in earthworms;</li> <li>- population assessment of chronic exposure to earthworms;</li> <li>- secondary poisoning;</li> <li>- population effects on higher trophic level;</li> </ul>
Model	Developed as tool for scientist, no public available version
Substances	PODYRAS may be applied to: <ul style="list-style-type: none"> <li>- heavy metals (validated for Cd, Cu);</li> <li>- site specific mixtures</li> </ul>
Ecological	Terrestrial food-chains with earthworms in the basic node
Acceptance	High scientific quality based on Dynamic Energy Budget theory and recent developments in population dynamics.
Predictive/Comparative	PODYRAS can be used both for comparison and predictions.
<b>Scale</b>	
Time	The time scale of the model ranges from months to ages, depending on the generation time of the objective species.
Space	Space is implicit in the model
Restrictions or possibilities for extrapolation to other scale(s) (time, space)	No restrictions
<b>Realism</b>	
Empirical/Theoretical basis (i.e. is the model based on a statistical or on a mechanistic approach?)	PODYRAS is a mechanistic model, witch input parameters are obtained by empirical measurements.
Missing processes	- demographic and environmental stoichasticity.

Assumptions (and their consequences)	Several assumptions form the foundation of this model. These assumptions have described in detail in various papers (see below).
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<b>Input/output</b>	
Minimum requirements	Site or pollutant specific vital rates of earthworms, predation rate, soil concentrations, diet composition predator
Optional	Earthworm densities and toxic load, soil characteristics
Benefit of collecting more data / Data efficiency	Collecting more data should improves the applicability of the model
Data availability	Low, input data from laboratory studies with a duration of minimal 6 months
Range of parameter values that may be entered to obtain reliable results	Not relevant
Internal parameters (units)	Dynamic Energy Budget parameters
Which parameters are estimated within the model that could have been obtained by other means (i.e. empirical data)?	None
Output variables (output)	Population growth rate ( $y^{-1}$ ) equilibrium population density ( $\#/area$ ), equilibrium population biomass ( $g/area$ ) time to detrimental effects (kidney lesion)
Graphics/Numerical output	The model returns both numerical and graphical output data.

<b>Uncertainty</b>	
Model outcomes	Qualitative behaviour of model uncertainty quantified. Uncertainty in predictions remain difficult to quantify given uncertainty in input parameters
Is reduction of uncertainty achievable?	Yes.

<b>Validation</b>	
Status	Population growth and development validated for Cu.
Scope of validation (representativeness validation study)	The model has been validated for comparative soils
Documentation of validation	Well-documented (see below).

<b>Feasibility of model</b>	
Reproducibility of results (Consistency & Variability)	PODYRAS is a deterministic model.
Flexibility	The model may easily be adjusted to specific aims and circumstances.
Complexity/Comprehensibility	Complete model has to be run by experts, but individual equations can be used by scientists from publications.
Model availability	Not available for third parties
Calculation time	Moderate.

<b>Alternative models</b>	
Alternatives	Up to date no alternatives.
Links/Co-operation with other models:	Can be linked with soil concentration models to project effects on large scales
Reputation in comparison with alternatives:	Not relevant

<b>Development</b>	
Options for improvement(s):	Currently pollutant availability depending on soil characteristics is included

Future plans:	Future development: -model parameterization for other pollutant e.g. Zn -development and inclusion of a soil functioning model -Including demographic and environmental stoichiasticity in basic earthworm model - application to other protected species which feed on earthworms
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#### Documentation

Klok and De Roos (1996); Klok et al. (1997); Latour et al. (1997); Klok et al. (1998); Klok and De Roos (1998); Klok et al. (2000, 2000b); Klok (2000); Bosveld et al. (2000); Kros et al. (2001c); Kros et al. (2001a), Boudewijn et al. (2002); Brink et al. (2004); Klok et al. (Submitted).

### 4.3.4 CATS

The food web model *CATS* (Contaminants in Aquatic and Terrestrial ecoSystems) is built as an integrative model to answer questions on the dynamic impact of toxicants on fluxes of contaminants, nutrients and biomass and species interactions. It has been used to study bioaccumulation, the impact of toxicants on species interactions and ecosystem function Traas et al. (1996); Traas et al. (1998a).

The model calculates the dynamic energy flows and competition between species utilizing the same resource within either terrestrial or aquatic food webs and can include top predators. It is firmly rooted in the tradition of ecological water quality models on eutrophication (Janse et al., 1997). The following CATS-models have been constructed (by T. Traas):

1. CATS-1 is for meadows
2. CATS-2 is for rivers or lakes
3. CATS-4-9 are for different substances in microcosms
4. CCOSM is the final model only for microcosms

The general description is valid for all models; documentation points to relevant documents.

Scope	
Use in policy making	No. Developed to predict ecological (side) effects of pesticides on populations in food webs
Model	CATS family
Substances	Metals, organic compounds.
Ecological	Terrestrial (grassland), aquatic (rivers, lakes, indoor test systems)
Acceptance	Not accepted for regulatory decisions. Used in scientific research
Predictive/Comparative	Both

Scope	
Time	Depends on dynamics of the process. Both for short-scale events (hours to days) as long-range prognosis (years).
Space	m <sup>2</sup> scale, homogeneous box model (zero dimensional). Contains litter-layer and soil or water-sediment layers.

Realism	
Empirical/Theoretical basis (i.e. is the model based on a statistical or on a mechanistic approach?)	Mechanistic dynamic model.
Missing processes	Intra-functional group competition and replacement.

Assumptions (and their consequences)	Species are lumped in functional groups, according to similar ecological function and/ or feeding preferences. Parameter estimates for functional groups are based on the most dominant species within the group. Without a statistical treatment of species sensitivity towards toxic substances, species within the functional group all have the same sensitivity.
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<b>Input/output</b>	
Minimum requirements	<ul style="list-style-type: none"> <li>- Fate parameters: sorption, degradation, volatilization</li> <li>- Ecological parameters : growth, respiration, mortality, feeding rate, food preferences, half-saturation rate, carrying capacity</li> </ul> Toxicological parameters: dose-response curve (slope, midpoint (LC50 or EC50)).
Optional	
Benefit of collecting more data / Data efficiency	To pinpoint dynamics of the effects of toxicants on functional groups, weekly sampling is best. The model is data and resource intensive.
Data availability	Depends on study and data set. Generally good for controlled (microcosm) experiments.
Range of parameter values that may be entered to obtain reliable results	See publications (section 10).
Internal parameters (units)	Mass-balance driven model; mass transfer is in either $\text{g biomass.m}^{-2}.\text{d}^{-1}$ or $\text{g toxicant.m}^{-2}.\text{d}^{-1}$
Which parameters are estimated within the model that could have been obtained by other means (i.e. empirical data)?	Ecological rates (growth, respiration, ventilation, feeding rates) can be estimated with allometric relationships, but can be measured as well.
Output variables (output)	Biomass and body burdens of functional groups in time, fate of chemical in environment, effect of toxicant on species.
Graphics/Numerical output	Both

<b>Uncertainty</b>	
Model outcomes	Contains uncertainty due to different sources: Biological variability, uncertainty about processes (model and fundamental uncertainty).
Is reduction of uncertainty achievable?	Yes. Depends on data availability and reducing model complexity. See Traas et al., 1995.

<b>Validation</b>	
Status	Not validated on external data; calibrated on experimental data
Scope of validation (representativeness validation study)	
Documentation of validation	

<b>Feasibility of model</b>	
Reproducibility of results (Consistency & Variability)	Good for normal use. No experience with 'outside use'.
Flexibility	Large. Can be adapted to different food webs.
Complexity/Comprehensibility	Relatively high complexity, to achieve high ecological realism
Model availability	Not available as stand-alone application. Available as model code for research purposes
Calculation time	Several minutes. Not critical for application.

<b>Alternative models</b>	
Alternatives	AQUATOX, IFEM (See Koelmans et al., 2001)
Links/Co-operation with other models:	Conceptually similar to AQUATOX
Reputation in comparison with alternatives:	See Koelmans et al, 2001



<b>Developments</b>	
Options for improvement(s):	Addition of user-friendly shell/ reprogramming for stand-alone application
Future plans:	Depend on user-demand

<b>Documentation</b>	
Traas and Aldenberg (1992); Traas and Aldenberg (1993); Traas et al. (1994); Traas et al. (1995a); Traas et al (1995b); Traas et al. (1996); Traas and Aldenberg (1996); Traas et al (1998b); Traas et al. (1998a); Traas et al. (2005)	
Modellen review (oa. CATS, AQUATOX, IFEM): Koelmans et al., (2001)	

## 4.4 Expert models

### 4.4.1 PERPEST

*PERPEST* (Predict the Ecological Risks of PESTicides ) is an expert based effect model in the sense that it basis its prediction on the results of real data in aquatic ecosystems. The *PERPEST* model is based on the *BASIS* methodology, see Van Nes and Scheffer (1993), in the sense that it searches for analogous situations in the database and calculates a prediction using weighted averaging of the effects reported in most relevant literature references.

One of the attractive features of the basis of *PERPEST* is that it can learn: i.e. the more information and/or experimental results are incorporated in the program, the better its predictions will be.

The *PERPEST* model is made for the prediction of the effects of a certain pesticide on various (community) endpoints, but the model can easily be expanded to other chemicals. For the *PERPEST* version of *BASIS*, a literature review of freshwater model ecosystem studies with insecticides and herbicides was performed to assess the  $NOEC_{ecosystem}$  for individual compounds and to evaluate the ecological consequences of exceeding these standards. Effects on various endpoints (e.g. community metabolism, phytoplankton, macro-invertebrates) were classified according to their magnitude and duration. This literature review resulted in a database containing the effects of 18 herbicides and 21 insecticides. In total 90 experiments (42 herbicide, 48 insecticide) were evaluated, resulting in 317 cases (155 herbicide, 162 insecticide). In this model one can enter the relevant properties of the compound, concentration and type of ecosystem to be evaluated (by P. van den Brink, version Van den Brink et al., Alterra, 2001).

*PERPEST* results in a prediction showing the probability of effects on the various groups. The model is integrated in a user friendly user interface. An example of output has already been shown in Figure 6.

<b>Scope</b>	
Use in policy making	<i>PERPEST</i> can be applied for the ecosystem-level risk assessment of pesticides, for their registration and to evaluate chemical monitoring data (e.g. in the light of the water framework directive)
Model	Freely available with Graphical User Interface
Substances	Pesticides
Ecological	Yes includes indirect effects
Acceptance	Yes, it is scientifically accepted
Predictive/Comparative	Both

<b>Scale</b>	
Time	weeks to year
Space	ditch, streams

<b>Realism</b>	
Empirical/Theoretical basis (i.e. is the model based on a statistical or on a mechanistic approach?)	Empirical
Missing processes	Connectance between ecosystems, mixtures
Assumptions (and their consequences)	Results of mesocosm experiments are representative for the real world

<b>Input/output</b>	
Minimum requirements	Type of pesticide (herbicide or insecticide), nominal concentration and toxicity to standard test organisms
Optional	Pesticide fate characteristics, mode of action, molecule group, name of substance, hydrology of water body, type of exposure,
Benefit of collecting more data / Data efficiency	Yes, since it is an empirical model it “learns” when more data are incorporated
Data availability	Large
Range of parameter values that may be entered to obtain reliable results	See manual
Internal parameters (units)	Concentration (µg/L) Pesticide name (-) Cas number (-) Type of pesticide (insecticide, herbicide) Mode of action (-) EC50 (µg/L) DT50 (days) Henry coefficient (Pa m <sup>3</sup> /mol) K <sub>om</sub> (L/kg) Number of effect classes (3, 5) Exposure (single, multiple) Hydrology (Stagnant, Flow-through) Weighing factors (-)
Which parameters are estimated within the model that could have been obtained by other means (i.e. empirical data)?	Since it is an empirical model this is not possible
Output variables (output)	Chances of no, slight or clear effect on 8 grouped endpoints. Differentiation between short-term and long-term clear effects is optional
Graphics/Numerical output	Both

<b>Uncertainty</b>	
Model outcomes	Yes, confidence intervals of probabilities of effects are provided
Is reduction of uncertainty achievable?	Yes, by enlarging the data base of PERPEST

<b>Validation</b>	
Status	PERPEST is validated by some observation done in the field
Scope of validation (representativeness validation study)	Many papers deal with the representativeness of mesocosm experiments for the real-world and it is generally accepted that mesocosm experiments are representative
Documentation of validation	Many guidance documents

<b>Feasibility of model</b>	
Reproducibility of results (Consistency & Variability)	Yes

Flexibility	Not so flexible, incorporated in GUI
Complexity/Comprehensibility	Not so complex, easy to use
Model availability	Freely available via <a href="http://www.perpest.alterra.nl">www.perpest.alterra.nl</a>
Calculation time	Seconds

<b>Alternative models</b>	
Alternatives	Food web models
Links/Co-operation with other models:	No
Reputation in comparison with alternatives:	Good, food-web models are more difficult to parameterise and use

<b>Development</b>	
Options for improvement(s):	Pesticide mixtures, Fungicides
Future plans:	Include fungicides and pesticide mixtures

<b>Documentation</b>	
Van den Brink et al. (2002b); Van Nes and Van den Brink (2003)	



## 5. Towards improved risk management

### 5.1 Policy targets, models and measurements

This report has shown a broad group of protection targets (water, soil, sediment, nature), or risk management decisions (water, sediment and soil sanitation and species and area protection plans). Nonetheless, there are large similarities accross policies in the way that scientific methods make use of models and approaches to measure the role of toxic impacts – alone, or in combination with other stressors. Fate and exposure models are applied to predict ambient or local toxicant concentrations and the magnitude of sorption to the matrix of exposure in the different exposure media (not specifically addressed, but see e.g. De Zwart et al., 2004). Statistical effect models are applied for water, sediment, soil protection and for assessing the need for risk management (*IRAsed.v1*, Posthuma) and sanitation urgency (SUS, see also Koolenbrander 1995). Mechanistics-based effect modelling ranges from population modelling for target species to community-level assessments of food-chain transfer and effects of compounds in water and soil. Apparently, the translation of generally formulated policy and risk management problems and regulatoty desires into scientifically formulated ‘rulers’ to quantify whether the targets are reached, has yielded a small set of basic models, that is:

- fate and exposure models to predict exposure, including food-chain and food-web models in which the exposure of higher organisms is mediated through biota (prey species)
- statistically-oriented effect models
- mechanistically-oriented effect models

When a certain “ruler” has been designed, it can be used for preventive policies (e.g., the HC5 derived from an SSD), for decision-making on curative problems (e.g. HC50 from the same SSDs to trigger investigations into remediation urgencies (Koolenbrander, 1995)) and also probably for risk management decisions of persistent environmental problems like the problem of handling slightly contaminated sediments (Posthuma et al., 2005).

Figure 2 focuses, amongst others, on this first translation step. The first key issue of this Figure is, that a clear definition of the policy problem is needed to derive an appropriate scientific ruler to quantify impacts – that is needed in order to make policy discrimination between unacceptable and acceptable impacts.

Models are often used to define the scientific “ruler” in the translation from policy problem to scientific assessment. However, it should be acknowledged that models are not the *sole* and unique approach to address the problem. Next to models, the scientific “ruler” can consist of only measurements, or a mixture of models and measurements. An example of the latter approach is the so-called Triad approach. The Triad-approach as being developed for soil risk assessment is based on a Multi-Criteria Analysis approach, whereby the guiding principle is the concept of Weight-of-Evidence (WOE). In three Triad-“legs”, the approaches are (1) a chemistry-based analysis of risks, (2) a bioassay-based analysis of (mixture) effects to biota exposed under controlled conditions to the sampled contaminated media and (3) a field inventory of visible damage in the field ecosystems. When all three types of approach point in the same direction, even when only very quick-and-dirty methods are applied for reasons of resource limitations, the WOE-principle would state that the situation is clear. The management decision to be taken further only asks for cut-off levels as to when the

assessment can be stopped with sufficient certainty, or when a next tier is to be executed (De Zwart et al., 1998).

Whether models, measurements or combined (WOE) approaches are the most prominent candidate to use for an environmental problem is a matter of choice. However, one should consider that it is eventually modelling that has yielded the EQCs and that exposure at low concentrations, even to mixtures, may not yield easily observable effects in bioassays or field inventories. An example of the difficulties encountered by using e.g. bioassays in the judgement of environmental quality is provided by a field study on sediment deposition on land. Soil samples consisting of soil mixed with relatively highly contaminated sediment didn't show easily interpretable effects in a set of bioassays (Seuntjes et al. 2004). Either modelling or measuring as a method for assessment can be chosen on the basis of the contamination level (see Figure 10). When considering the selection of study sites for SSEO, where the target was to find “grey veil” locations, it is logical to (at least) address the policy problems by modelling analyses.

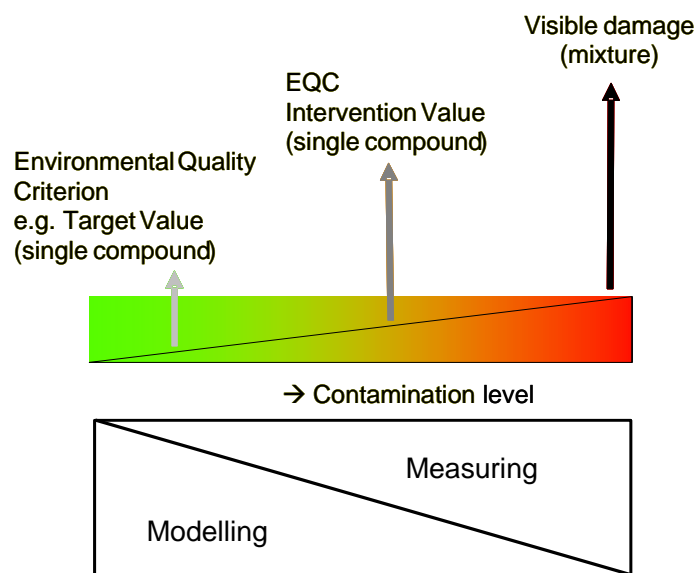


Figure 10. The application of Models and/or Measurements as methods to analyse a contaminated system is related to the exposure level.

*At the Target Value (a result of modelling, see e.g. Figure 3), it is unlikely that simple effect measurement will show adverse effects in bioassays or field inventories. At the highest exposure levels, modelling is unnecessary, since effects can be seen by visual inspection of a site (e.g., the barren area of Maatheide, Belgium).*

## 5.2 Selection of data and models

The selection, availability and quality of input data are of major importance to run models. Model outcomes depend both on the “modelling engine” and the “fuel” provided by the data. It is common that practical risk assessment applications based on modelling depend on existing data sets, not on data collected for the specific purpose. Whether or not the output of models is meaningful for effective policies depends on the appropriateness of the data to the assessment problem and on the degree of validation of the model. It may be obvious that wrong model choice or good models applied to a problem for which use is inappropriate, can

easily lead to mismanagement of risks. Furthermore, it may be obvious that non-relevant data give a “disturbed” view, even if the best model is applied.

Models, especially lower-tier models, are designed in view of a balance between accuracy in prediction and technical feasibility and aspects such as operational ease and costs. The principle of parsimony, also known as Ockham’s razor, is usually applied. That is: models in lower tiers should be formulated as simply as possible without losing their ability to make the required predictions. As an example, general environmental protection could be based on mechanism-based population models for surrogate species that represent all relevant groups of species in an environmental compartment, but this approach has never been chosen. The probable reasons are, that running such models would ask for input data that do not exist for a wide range of chemicals and that the limited set of species for which population models can be run were not considered to represent the protection problem as a whole. Instead, simple models like the lowest NOEC divided by a safety factor, or a low percentile of a sensitivity distribution (e.g., the HC5) have been chosen as parsimonious alternatives, whereby the approaches yield the desired output for many compounds. For certainty, various methods are used complementarily to each other. For example, the legislative risk limit chosen for general soil protection is the lowest of a few modelling exercises, namely of that for structural effects on soil communities in comparison to that for functional effects (Sijm et al., 2002).

In the next step of Figure 2, the link needs to be made between the scientific ‘ruler’ that was designed to address the policy problem and the true occurrence of undesired effects in the field. When the ‘ruler’ was constructed by a model (or even by various optional models), the key question of validation comes up: “does the chosen ruler, as defined by model output, accurately predict the level of adverse effects in field ecosystems?”. And, when various models can be used to address a risk management problem, the additional question is: “do simple models equally well predict those adverse effects as complex models?”. If that would be the case, the policy preference could generally be biased to the simpler models. If it wouldn’t be the case, it can be envisaged that the toolbox of assessment models should have a tiered structure, with the simpler models for a conservative assessment of generic-type problems and the more complex models for more specifically described problems. Also nature policies follow in principle a tiered approach. Since the objective is usually not the complete ecosystem but rather the viability of a specific species which is stressed by a multitude of factors of which pollutants are only one, the tiered approach differs from that of environmental policies. As a first tier the probability that the pollutant reaches the species should be assessed. For pollutants which reach species through the food-chain information on the food ecology of the species and levels of pollutants in the food are used and simple accumulation models, e.g. as exemplified in the badger (Klok et al., 2000). If indeed pollutants reach the target species, more complex models can be applied.

In some cases, low and high tiered approaches can be followed with the same basic tools. To illustrate this, the RIVM-e-toxBASE (Wintersen et al., 2004) contains data from which sub-selections can be made to create SSDs. One can select a relatively large subselection of data of acceptable scientific quality for general assessment problems, or high-quality and consciously selected data for specific assessment problems. By doing so, different tiers can be addressed for different problems (Posthuma et al., 2002a). The RIVM e-toxBASE is programmed in such a way that subselections can easily be made, in accordance with the assessment problem and in line with the approaches followed in *IQtox*. The tiering is executed, in such cases, in the selection of input data (specific or generic) rather than in the modelling itself.

### 5.3 Model validation

The next link step in Figure 2 (page 14) addresses the validation issue in more detail, viz. the link between assumed mixture effects in the field and the quantification of those effects. The identification of effects in field situations is difficult due to (1) the presence of mixtures of toxic compounds, (2) the true level of exposure to those compounds, given the sorption characteristics of the matrix and the media, (3) the measure of effect that is to be defined (e.g., population density at the community level, or the Shannon-Wiener Index to quantify community-level effects), (4) ecological interactions amongst species (both in the transfer of toxic compounds [food-chain] as well as in the form of competition or predation) and (5) the presence of multiple-stress conditions (changes in the field are the net result of all factors, not only toxicant exposure). Therefore, the diagnosis of field effects is generally considered a complicated matter (Suter et al., 1993).

In the diagnosis of field effects, the researcher defines one or more measures of effects, as exemplified above. Evidently, the measures of effect need to be associated to the risk management problem. In the case of target species, the definition of the measure of effect is relatively simple, e.g. population size, whereas in the case of community-level parameters complications may arise. For example, one can choose for an overall parameter (like the Shannon-Wiener index for biodiversity, the data for species are compiled into one number, the index value) or for the response curves of all species separately. The latter parameter is evidently much more sensitive than the composite parameter, because it is explicitly shows the change in abundance of the most sensitive species. Examples of validation studies in which the diagnoser offered various measures to quantify field effects are Smit et al. (2002) and Klepper et al. (1999).

The key issue of the second phase of the SSEO-integration project is the study of model validation, especially for the models that are used in Dutch environmental policy. The following provisional Table of Options has been derived by merging the Model Inventory (section 3.4) with the Project Descriptions of the research projects on field effects funded by the SSEO-program. The SSEO projects are depicted in the columns and the models that can be applied are depicted in the rows.



*Table 2. Example of provisional matching the inventory of models to the data sets collected in SSEO-program (scientists are made anonymous).*

An 'x' sign indicates good opportunities for validation, a zero indicates that these opportunities are likely good (further evaluation needed). V, B and A are research sites for the SSEO-program, viz. V=Ronde Venen, B=Biesbosch and A=Afferdensche en Deestse Waarden. Note that during the research progression, the matrix will change according to collaborations being started.

Model type	Model name	Scientists responsible for the different projects																				
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
Exposure	Various																					
Statistics-based	ETX-2004	x	o	x	o		x	x	x	x	x		x		x		x	o	o	x	x	
	OMEGA123					x	x	x	x	x	x				x				o	x		x
	IQ-TOX	x	o	x	o	x	x	x	x	x	x				x			o	o	x		
Mechanism-based	HERBEST															x			x	x		
	OMEGA45		x			x	x	x	x	x			x				x			x		x
	PODYRAS		x	x					o	x		x		x			x				x	
	CATS		o		o	x	x		x	x			x		x	x		o	o	x		
Expert system	PERPEST															x				x		
Research location SSEO		V, B,A	V	V	V	B	B	B	B	B	V	V	A	A	A	A	A	A	A	A	A	A,B

To investigate robustness of the model in prediction accuracy for different situations, the horizontal sets of validation researches are important. A robust model would predict responses accurately, independent of the site and specific conditions. The vertical sets of optional validation researches is important to investigate whether tiering is possible and for the sake of using the simplest model for the sake of practicality. In this way, the advantages and disadvantages of each model (higher tier might have data input problems or lower tier might be too simplified) can be seen. Suitable models will be scientifically compared based on the output they generate for the SSEO datasets. These actions result in a conclusion on having insight in the most optimal situation for environmental risk modelling. This might be a compromise between most accurate model (desiring many input parameters) and the most generic model giving simplified predictions, however is mostly applicable to each situation because of few data requirement.

Validation research may result in different conclusions: the model can be adopted (for certain purposes), adapted (when accuracy is improved upon model improvements) or abandoned (when insufficiently accurate). The problem being investigated in the SSEO-program is difficult and consists of the steps identified in Figure 2. Nonetheless, the planned activities are feasible as long as that there are good field data - it is namely likely that various models can be run anyway on the basis of ambient concentrations only. As an example, the Appendix shows how the steps depicted in the Figure are worked out. The example is taken from ongoing research works at RIVM, concerning investigations outside the SSEO-sites.

## 5.4 A toolbox for regulations and risk management

### 5.4.1 What is currently in the toolbox?

The tools that are currently used for the underpinning of Dutch environmental policies consists of both fate-, exposure- and effect models. As yet, instruments for the toolbox are

used for a wide array of risk assessment problems and they appear to be specifically adapted and tailored to the specific problems. The risk manager currently needs to decide on a case-by-case basis which combination of tools accurately fits to the situation. Finally, there is limited coherence between the lines along which the models are further being developed, since they originated in different institutes, were designed for (slightly) different problems and evolve further in different policy frameworks. In summary, one cannot currently speak of a Dutch toolbox for environmental risk assessment of toxic compounds. The toolbox concept presupposes a designed box in which the tools are ordered and where for every tool there is a specific problem and *vice versa*.

#### **5.4.2 Towards a toolbox**

The existence of differences in approaches addressing the specific policy problems does not mean that the current situation is bad. It is not bad that models are tailored to the wide array of problems that needed to be tackled. However, some guidance in the design and use of tiered risk assessment systems may be of substantial value for maintaining support for the use of formal risk assessments. It should be avoided, by the scientific community of risk assessors, that one policy question can result in completely different answers. This would undermine credibility of risk assessors and eventually of risk managers, i.e., the environmental policy itself. Evidently, this needs to be avoided. It should be noted that this problem is currently of key interest to the European Union too, in view of the issue of Risk-Based Land Management (RBLM, Carlon [EU-research, Ispra], pers. comm.).

Improving on the transparency of the tiering system may be of great help. Currently, various efforts are underway to guidance on the use and interpretation of risk assessment models in a tiered system. Efforts in this direction are made by the Dutch government, as shown by this report and as shown by current incentives for defining the science-basis for the assessment of soil protection under the auspices of VROM-BWL (pers. comm. Swartjes [RIVM]). In the international context, a book will soon be published on the use of extrapolation models in the risk assessment of toxic compounds (Solomon et al., 2004). All these efforts mean, that the governmental institutes will likely create a toolbox for ecological risk assessment soon.

#### **5.4.3 What is currently missing from the toolbox?**

Two major items are missing in the general outline idea of the toolbox, the exposure models and the rules for use.

Although this report has addressed effect models specifically, there are also exposure models. These models need to be part of the toolbox, since risk is (by definition) a matter of exposure and sensitivities and effects. In the validation studies of the second phase of the SSEO-integration project, exposure models will likely thus also be tested.

Rules for using the different tools can be set when the validation activities have shed light on the accuracy of prediction of different models. As yet, such rules are lacking. The SSEO-program may be of help in identifying not only how the toolbox can be formatted, but also which use limitations one may set to the different models. This issue will be addressed within the second phase of the Integration-project of SSEO.

As stated in section 2.4.2, Nature policies deal with a multitude of stress factors of which pollutants are only one. The toolbox provides useable models for species that are connected with earthworms in their food-chain, species like shrews, badgers and meadow birds which

directly feed on them but also predators higher in the food-chain such as barn owls. With the existing model version both direct (risk of poisoning) and indirect (food shortage) of heavy metals can be calculated for badgers and godwits. To include other species the modelling framework should be extended. It may be that, given the multitude of stress factors, pollutants are negatively affecting only to a limited extent the viability of 'higher' species. The models in the toolbox may in such a case serve as a warning signal. If this warning signal gives a red alert more complex models should be used.

Finally, there are some further needs. The most important one is *experience*. When a toolbox is to be used with success, the major issue is that it effectively discriminates between unacceptable and acceptable risks and effects, which is a policy choice. Today, some tools are still in their infancy and although they are scientifically well-underpinned regarding their principles, their cut-off values still need to be established. This need is urgent for e.g. the soil Triad approach, especially when considering the need for a 'quick version' that can help to identify sanitation needs under the new soil policies (VROM, 2003) on the basis of minimal investment (time, money), given that the inventory of workloads has identified various hundreds of thousands of potential sanitation sites (Kernteam Landsdekkend Beeld, 2004). Experience does not compile itself. Arrangements are needed to create 'self-learning systems', like e.g. the expert system applied in PERPEST, in which feedback from practical use of model results is fed back into the field of the model designers.



## 6. Summary of conclusions

### Regarding the problem setting of this report (phase-1 inventory stage):

1. There are many environmental problems with toxic compounds. At many sites and for various compounds the environmental quality criteria for toxic compounds are exceeded. The presence of ecological risks is thus currently frequently hypothesized due to the presence of a so-called “grey veil of contaminants” and thus there are many cases of assumed affected species, species groups and ecological functions. This generally suggests a need for risk management, either preventive or curative (policies) and/or for further considerations on the meaning of this “grey veil” for exposed ecosystems (science).
2. The meaning of the grey veil for exposed ecosystems is rather unclear, since the number of studies executed so far is low, while other stress factors may mask or enlarge pollutant effects at contaminated sites. Hence, the relationship between the hypothesized grey veil and the occurrence of (unacceptable) field effects is unclear.
3. For proper risk management (policies), risk assessments should yield “valid” information (science). The validity issue concerns the question how the results of risk assessments relate to the true effects of toxic compounds in exposed ecosystems. This project will address this validity question in phase 2, for a selected set of models.
4. There is a wide variety of explicit risk questions, posed in the contexts of general environmental protection and of nature and water management. This report presents an overview of the relationships between these policy questions and the scientific approaches to solve those questions. The overview is illustrated by a selection of different policy questions and shows a set of models that play a role in current risk assessments.

### Regarding the approaches and limitations of this report

5. This report is the step-up (phase 1) towards a set of validation activities that will be undertaken (phase 2) in the context of the Stimulation Program Systems-Oriented Ecotoxicological Research, whereby results of risk assessment approaches (in this case: models) are confronted with field effect data (validation).
6. This report is a limited inventory, concerning the description of a set of models currently applied in risk assessments and the linkage of these models to the different policy problems. The validation studies are subject of subsequent works.

### Regarding models

7. Environmental Risk Assessment (ERA) can be done by models.
8. There is a spectrum of models available in The Netherlands to address the large variety of questions posed in the contexts of environmental, nature and water management.
9. A small set of basis models can be selected to cover the main “rulers” in ERA, that is
  - fate and exposure models
  - statistically oriented effect models
  - mechanistically oriented effect modelsAs such, the models described in this report fills a niche and they are regularly applied in policy and practice
10. Models require different degrees of additional calibration or validation. The SSEO program is an opportunity to carry out these calibrations and validations.

11. In the work following after this report, validation research will be performed, given some practical limitations, like a selected set of models and data.
12. As remark: models are certainly not the sole way to address problems. Measurements or combinations of modeling and measurements are the alternatives. The type of assessment problem (prevention, remediation) and the exposure level are factors that help to determine which approach to choose for a given problem.

**Regarding future developments**

13. Models and approaches can be brought together in a toolbox of models, with guidance on their usefulness for different problems and on their limitations. Tiering and parsimony are guiding principles for effective and efficient risk assessment, so that such a toolbox could contain multiple tools for one problem type: simple approaches with larger resulting uncertainty when possible, more complex approaches and specific answers when needed.
14. Usefulness and limitations of models in the toolbox can be, better than now, be judged from the results of the upcoming validation studies undertaken within the context of the SSEO-program.
15. Tailored and efficient development of models can be supported by early recognition of similarities across problem definitions on the one hand (problem definition, policy) and collaborations across research institutes on the other hand (scientific approaches, institutes).

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## Appendix 1. An example of model validation

### Introduction to a case study on model validation

Validation of model results will be the key issue of phase-2 activities in the SSEO-integration project and validation study results are key to the formulation of rules of application of models in the toolbox.

To illustrate the meaning of validation studies in this context, one example of such a study is shown. The example (stepwise) visualizes the issues captured in the Figure below and shows what type of results might be obtained.

The example concerns the statistics-based effect modelling for toxic compounds using the *IQtox* approach and is described by De Zwart et al. (2005 accepted) and Posthuma and De Zwart (In press) (block 2 in the Figure) and ecological diagnostic assessments (translation of the complex set of field phenomena of block 4 into a measure of effects that is specifically reflecting the toxicant stress, in block 3).

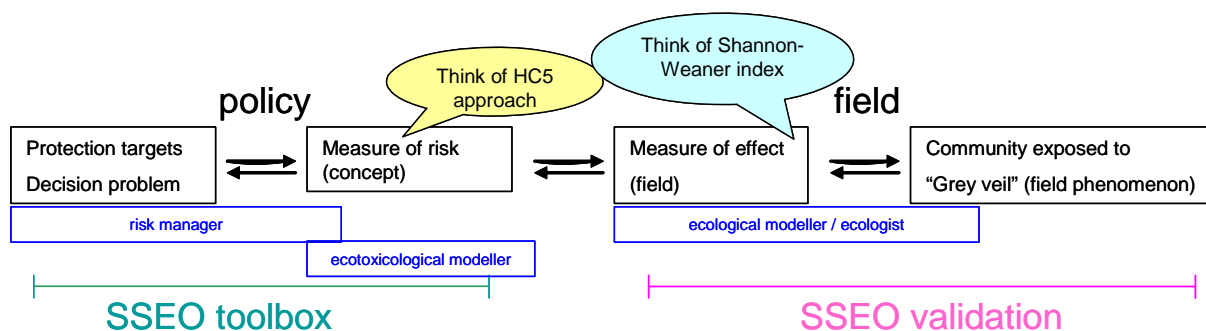


Figure A1: the example: condition of fish assemblages in Ohio rivers

### The problem in the field (box 1 in the Figure)

Fish assemblages in Ohio surface waters are known to be impacted by a broad variety of stress factors, amongst which physical disturbance (e.g., channellization), water-chemistry change (e.g., altered pH), waste-water treatment effluents and toxic compound mixtures.

Various studies have identified local impact magnitudes. However, it is only possible to apply expert judgement when the river manager wants to reduce local impacts. He is confronted with the question which of the stressors *locally* affects the local fish assemblages most: toxicants, or other stressors? Knowing impact is insufficient to know causes and causal analysis is needed for effective and informed decision making.

When it is a possibility that local river stretches are under stress of toxicant mixtures at low concentrations, expert judgement usually falls short. It is highly unlikely that expert judgement is sufficient to uncover a role of such mixtures; such judgement often only works for accidental spills in the river, where concentrations are high and suspect causes are easy to identify (e.g., a discharge point). Ecological data analysis is needed to disentangle the impact of toxic stress from the impacts of other stressors. This is done as described below.

### *Quantifying mixture risks in Ohio rivers (box 2 in the Figure)*

To diagnose the possible role of toxicant mixtures at low concentrations at all the different locations, the available monitoring database<sup>4</sup> of stressors and fish species abundances was analysed. By ecotoxicological modelling (using *IQtox*), measured toxicant concentrations in the river systems were re-calculated into the locally multi-substance Potentially Affected Fraction (msPAF), making use of the SSD-approach and established principles from mixture toxicology (De Zwart and Posthuma, in press). Whereas the separate compounds could not be associated to impacts due to statistical lack of power (each compound that is added as variable in a monitoring program reduces the statistical diagnosis power for all variables!), the msPAF appeared to show clear signal accross Ohio. That is: the model of SSD, in combination with exposure and mixture assessment rules, generated a singular parameter for toxic stress of mixtures.

### *Quantifying impact from field observations (from box 4 to box 3 in the Figure)*

The impact on fish assemblages was quantified using an ecological model, RIVPACS, addressing the presence or absence of fish species at the sampling sites. Based on a set of reference sites, the local fauna could be considered impacted or not, as compared to the set of reference sites. This ecological model is often used to quantify impact, but it is not possible to assign probable causes. Hence, fish census data (box 4, the raw field data) were translated by ecological modelling into local measures of effect (i.e., a quantitative measure of local impact). Next to the quantification of impact, the model also shows which species are expected – but absent and which species are present – but not expected. The identity of these species is of key importance for the last step of the analyses, merging impact quantification to a probably causal structure in the data set.

### *Validation of the toxic risk model against the measures of effect (do box 2 and 3 match?)*

Preliminary data treatment. The predicted risk is quantified by the local estimates of msPAF and the impact is quantified by RIVPACS. The impact is, however, not the sole effect of the toxicant mixtures and therefore, an additional step was made. In that step, the level of impact was studied as a function of all different possible causes. This resulted in the so-called Effect-and-Probable Cause Pie diagrams (De Zwart et al., in press) in which the pie size represents the local impact (measure of effect, box 3) and the slice size the probable cause (see Figures below for the principle and the mapped output for some rivers systems, respectively).

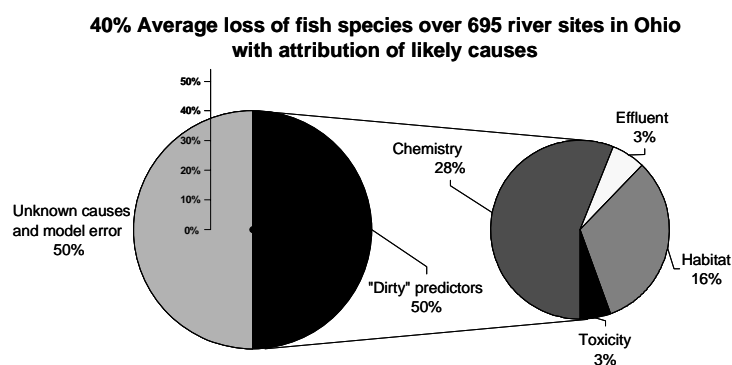
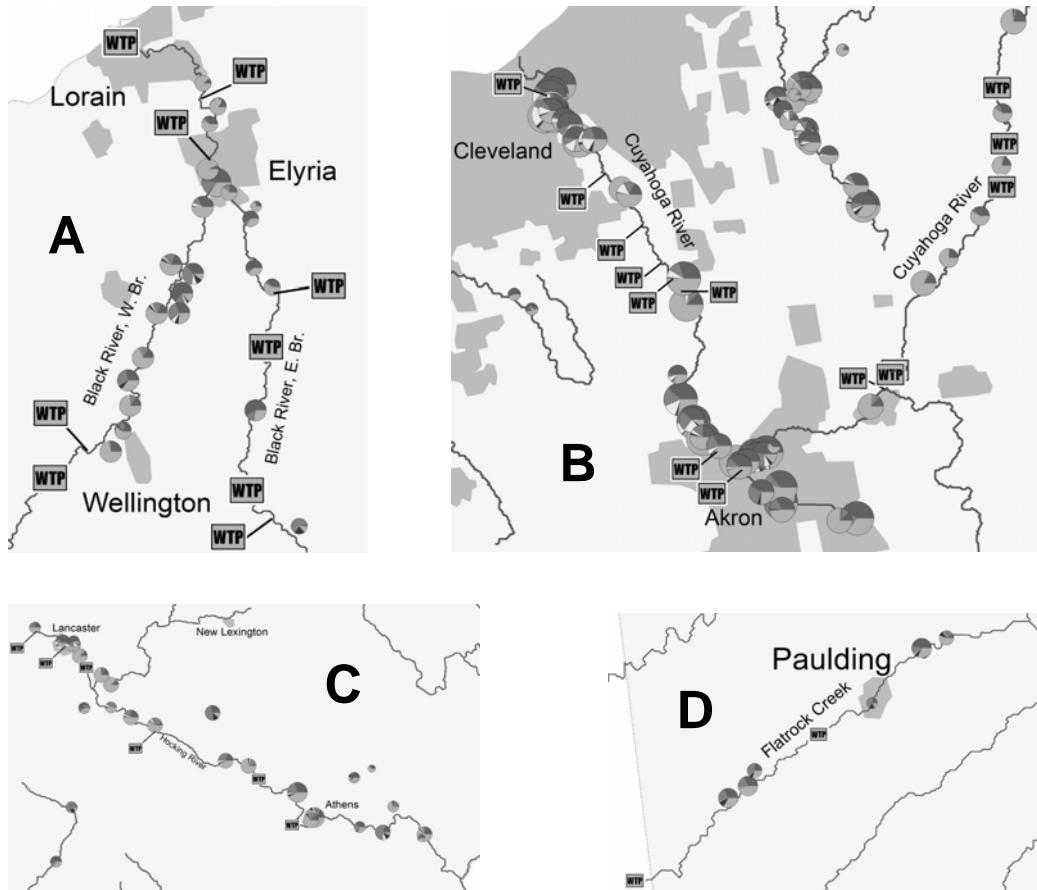


Figure A2: Example of an effect-and-Probable Cause Pie diagrams

<sup>4</sup> Compare: the SSEO field exposure and effect data sets



The slice size related to the presence of toxicants quantifies the impact of toxic compound mixtures on the local communities, proportional to the total impact. This means, a scaling is made by pie size and slice size, to yield a quantitative degree of impact assigned to mixture exposure, on a scale from 0 – 100. This is exactly the scale of msPAF. Hence, it became possible to map the impact of different stressors on local communities using GIS techniques (Figure below, the maps) and thereafter to study the accuracy of msPAF to predict local impacts on fish (Figure below, the line graph).



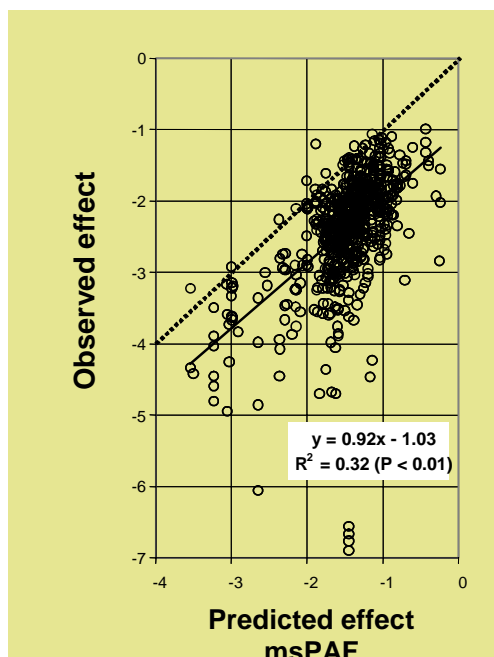


Figure A3: Example of predicted msPAF and observed effects in OHIO surface waters.

The latter Figure show that the predicted msPAF (based on SSD-modelling of *laboratory* toxicity data) has a straight relationship with the measure of effects in the *field* as obtained from the EPC-pie diagram calculations. The analyses also shows large impact of other stressors (vertical spread of data points at a single predicted msPAF on the X-axis), which means that predicting msPAF solely is insufficient for obtaining a view on local impacts. Such impacts may also occur due to e.g. the inundation frequency at the floodplains field site (ADW) or the heterogeneity and patchy contamination in the Ronde Venen and the Biesbosch, the three locaties of the SSEO program. The analyses of Ohio show that a multi-stress view is needed to understand the field phenomena.

Nonetheless, the Figure suggests that the SSD / msPAF methodology predicts the risks of contaminants in a linear way, with the following special notions:

- the association between predicted msPAF and observed impact assigned to mixtures is grossly linear (when modelled to all data points); this implies a gross prediction accuracy, so that high msPAF likely associates to high impact (as expected, but never shown)
- there are hardly any data points above the 1:1 hypothetical line; this implies that the msPAF based on EC50 data as used in this assay apparently gives the upper limit of impact. In none of the cases the loss of diversity is larger than the proportion predicted by the msPAF<sub>EC50</sub>
- the observed line is below the hypothetical 1:1 relationship, which relates to the fact that species are lost due to another stressor and consequently the lost of species cannot be accounted to the toxicant anymore. Eventhough the toxicant levels would have had mortality effects on the species if the other stressor to which the species was more sensitive was not there.

#### Remarks and conclusions

In this example, validation of the SSD-model was possible by combination of knowledge of different disciplines.

- An ecologist covered the translation of assumed field effects into measures of effects (box 4 into box 3), via the ecological “tool” of RIVPACS modelling.
- Ecotoxicological modelling was needed to cover the translation of the assessment problem (do toxic compounds matter?) into a measure of risk (box 1 into box 2).
- Collaboration between all parties allowed for construction of the EPCs and thereafter the quantification of field effect levels assigned to toxicants.
- Only the latter allows for matching model predictions to field observations and thus policy targets to field phenomena.

An open question remains: which of the local systems can be considered ‘stable’, which ‘unstable’? This may be a key question to link box 1 to box 4 by ecological- and policy motives. Evidently, an unstable system has passed an ecology-based critical limit (rather than a ‘just-set’, or derived or hypothesized critical limit).

Phase 2 of the SSEO- integration project might result in validation efforts like the case study of Ohio.